

STIC Search Report

EIC 1700

STIC Database Tracking Number: 186748

TO: Rip A Lee
Location: REM 10A24
Art Unit : 1713
May 4, 2006

Case Serial Number: 10/525929

From: Mei Huang
Location: EIC 1700
REMSSEN 4B28
Phone: 571/272-3952
Mei.huang@uspto.gov

Search Notes

Examiner Lee,

Please feel free to contact me if you have any questions or if you would like to refine the search query,

Thank you for using STIC services!

Mei Huang



SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: RJP A. Lee Examiner #: 78680 Date: April 24, 2008
 Art Unit: 1713 Phone Number: 2-1104 Serial Number: 101525,929
 Mail Box and Bldg/Room Location: RM 10A24 Results Format Preferred (circle): PAPER DISK E-MAIL

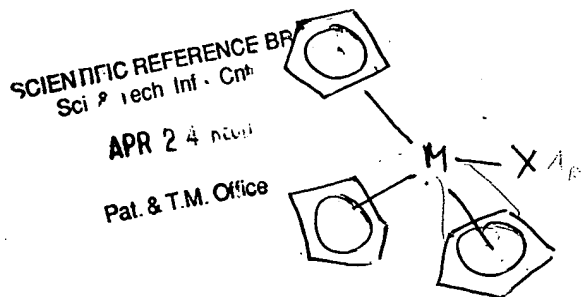
If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: NOVEL TRANSITION METAL COMPOUND
 Inventors (please provide full names): SEKI, T. TAKANASHI, T.
SHIMIZU, H. NAKAJIMA, K.
 Earliest Priority Filing Date: Oct 25, 2002

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

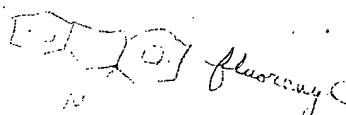
Please search for compounds having the following minimum structure:



M is Group 4 (Ti, Zr, Hf)

X - any ligand

cyclopentadienyls may be substituted, may also be indenyl



STAFF USE ONLY

Searcher: <u>MOH</u>	Type of Search	Vendors and cost where applicable
Searcher Phone #:	NA Sequence (#)	STN <input checked="" type="checkbox"/>
Searcher Location:	AA Sequence (#)	Dialog
Date Searcher Picked Up:	Structure (#) <u>1</u>	Questel/Orbit
Date Completed: <u>5/4/06</u>	Bibliographic	Dr. Link
Searcher Prep & Review Time:	Litigation	Lexis/Nexis
Clerical Prep Time:	Fulltext	Sequence Systems
Online Time:	Patent Family	WWW/Internet
	Other	Other (specify)



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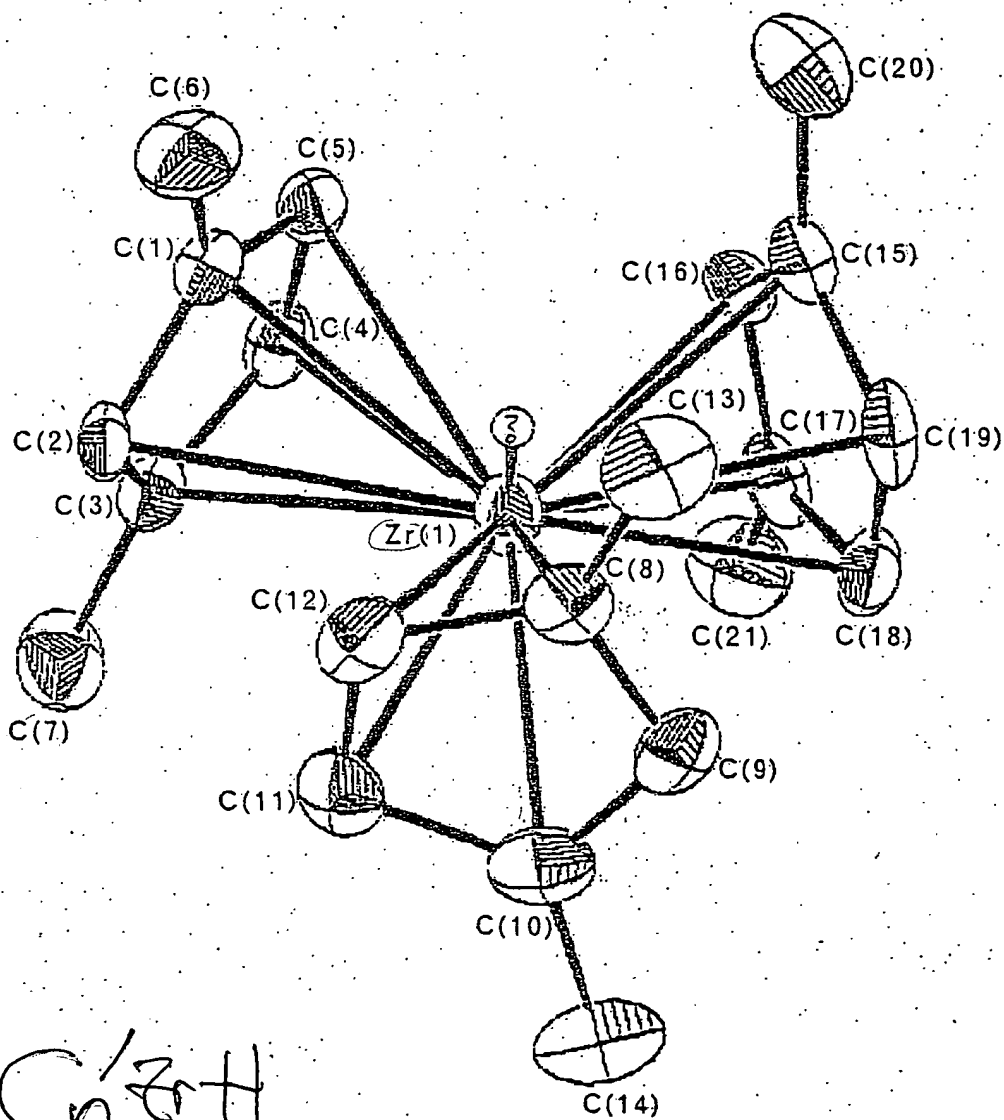
BIBDATASHEET

CONFIRMATION NO. 2836

Bib Data Sheet

SERIAL NUMBER 10/525,929	FILING OR 371(c) DATE 02/25/2005 RULE	CLASS 526	GROUP ART UNIT 1713	ATTORNEY DOCKET NO. 18644
APPLICANTS Takashi Seki, Kanagawa, JAPAN; Hiroyuki Shimizu, Tokyo, JAPAN; Tamotsu Takahashi, Hokkaido, JAPAN; Kiyohiko Nakajima, Aichi, JAPAN; Tetsuro Fukuda, Kanagawa, JAPAN;				
** CONTINUING DATA ***** This application is a 371 of PCT/JP03/13610 10/24/2003				
** FOREIGN APPLICATIONS ***** JAPAN 2002-311451 10/25/2002				
Foreign Priority claimed <input type="checkbox"/> yes <input type="checkbox"/> no 35 USC 119 (a-d) conditions <input type="checkbox"/> yes <input type="checkbox"/> no <input type="checkbox"/> Met after met Allowance Verified and Acknowledged _____ Examiner's Signature Initials		STATE OR COUNTRY JAPAN	SHEETS DRAWING 2	TOTAL CLAIMS 18
INDEPENDENT CLAIMS 1				
ADDRESS 23389				
TITLE Novel transition metal compound, catalyst for olefin polymerization and method for producing polyolefin				
FILING FEE RECEIVED 900	FEES: Authority has been given in Paper No. _____ to charge/credit DEPOSIT ACCOUNT No. _____ for following:		<input type="checkbox"/> All Fees <input type="checkbox"/> 1.16 Fees (Filing) <input type="checkbox"/> 1.17 Fees (Processing Ext. of time) <input type="checkbox"/> 1.18 Fees (Issue) <input type="checkbox"/> Other _____ <input type="checkbox"/> Credit	

Fig. 2



$C_{12}H_9$
B



STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact *the EIC searcher* or contact:

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

- I am an examiner in Workgroup: Example: 1713
➤ Relevant prior art **found**, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
(journal articles, conference proceedings, new product announcements etc.)

➤ Relevant prior art **not found**:

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to EIC1700 REMSEN 4B28

=> fil reg

FILE 'REGISTRY' ENTERED AT 17:25:08 ON 04 MAY 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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(FILE 'HOME' ENTERED AT 16:23:42 ON 04 MAY 2006)

FILE 'HCAPLUS' ENTERED AT 16:23:55 ON 04 MAY 2006

L1 15157 S SEKI ?/AU
L2 55873 S SHIMIZU ?/AU
L3 112152 S TAKAHASHI ?/AU
L4 37809 S NAKAJIMA ?/AU
L5 30177 S FUKUDA ?/AU
L6 3 S L1 AND L2 AND L3 AND L4 AND L5
L7 1 S L6 AND 35/SC
SEL RN

FILE 'REGISTRY' ENTERED AT 16:30:18 ON 04 MAY 2006

L8 22 S E1-22
L9 1 S L8 AND C21H28ZR/MF
L10 STR 683752-56-9
L11 STR L10
L12 0 S L11
L13 STR L11
L14 0 S L13
L15 STR L10
L16 11 S L15
L17 STR L15
L18 10 S L17
L19 STR L11
L20 5 S L19
L21 SCR 1845
L22 5 S L19 AND L21
L23 SCR 1918
L24 4 S L19 AND L21 AND L23
L25 1681 S L19 AND L21 AND L23 FUL
SAV L25 LEE929/A
SAV L8 LEE929AU/A
L26 109 S L25 AND B4/PG
SAV L26 LEE929S/A

*The Structure (See L19 on next page) and
Group 4 metals*

FILE 'HCAPLUS' ENTERED AT 17:19:48 ON 04 MAY 2006

SAV L7 LEE929AP/A
L27 81 S L26
L28 76 S L27 AND (1840-2002/PY OR 1840-2002/PRY)

FILE 'REGISTRY' ENTERED AT 17:23:10 ON 04 MAY 2006

L29 10 S L8 AND L26

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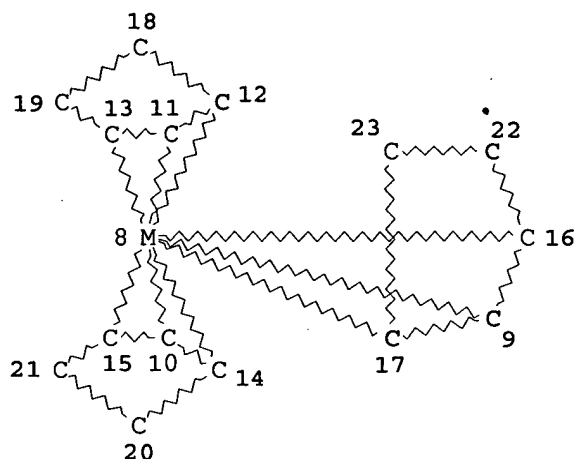
L30 2 S L29
L31 75 S L28 NOT L30

FILE 'REGISTRY' ENTERED AT 17:25:08 ON 04 MAY 2006

=> d l26 que stat

L19

STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L21 SCR 1845

L23 SCR 1918

L25 1681 SEA FILE=REGISTRY SSS FUL L19 AND L21 AND L23

L26 109 SEA FILE=REGISTRY L25 AND B4/PG

=> fil hcap

FILE 'HCAPLUS' ENTERED AT 17:25:21 ON 04 MAY 2006

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=> d l30 cbib abs hitstr hitind 1-2

L30 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

2006:11553 Document No. 144:70549 Ethylene polymers with improved moldability and mechanical strength and their manufacture. Shimizu, Hiroyuki; Fukuda, Tetsuro; Egashira, Toshiaki (Japan Polyethylene Corporation, Japan). Jpn. Kokai Tokkyo Koho JP 2006002098 A2 20060105, 35 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2004-181918 20040621.

AB The polymers satisfying the following (a) to (d) and having C1-20 short-chain branches and C≥20 long-chain branches are manufd. by polymn. of ethylene and optionally C3-20 α-olefins by the use of ≥2 metallocene catalysts contg. transition metal compds. having different reactivity to nonconjugated polyenes in the presence of ≤1 mol% (to ethylene) nonconjugated polyenes: (a) d. 0.880-0.970 g/cm³ measured based on JIS K7112, (b) melt flow rate (MFR) 0.01-100 g/10 min at 190° under 21.18-N load measured based on JIS K7210 table 1, condition 7, (c) difference between flow activation energy Ea (kJ/mol) and activation energy EaL (kJ/mol)

ΔE_a 1.5-12.5, where $E_{aL} = 24.3 + (1.4B + 5.2) + [1 - \exp(-SCB/10.7)]$ ($SCB = C1-20$ short-chain branch no./1000C; $B =$ carbon no. of $C1-20$ short-chain branch), and (d) elongation viscosity $\lambda_{max} \geq 1.2 \exp(0.721 + \Delta E_a)$.

Thus, 0.1 mmol tris(indenyl)zirconium hydride and 0.1 mmol tris(benzoindenyl)zirconium hydride were mixed with PhMe and 40 mmol (as Al) Me aluminoxane (MAO), stirred with 10 g SiO₂, and freed of solvent to give a solid catalyst. Ethylene was polymd. with 0.026 mol/mol-ethylene of 1-hexene contg. 2 mL/L 1,7-octadiene at 75° in the presence of the catalyst to give a polymer with MFR 7.8 dg/min, d. 912.8 kg/m³, Mw/Mn 2.87, SCB 24.3/1000C, E_a 37.4 kJ/mol, E_{aL} 34.0 kJ/mol, and λ_{max} 16.9.

IT 683752-59-2P

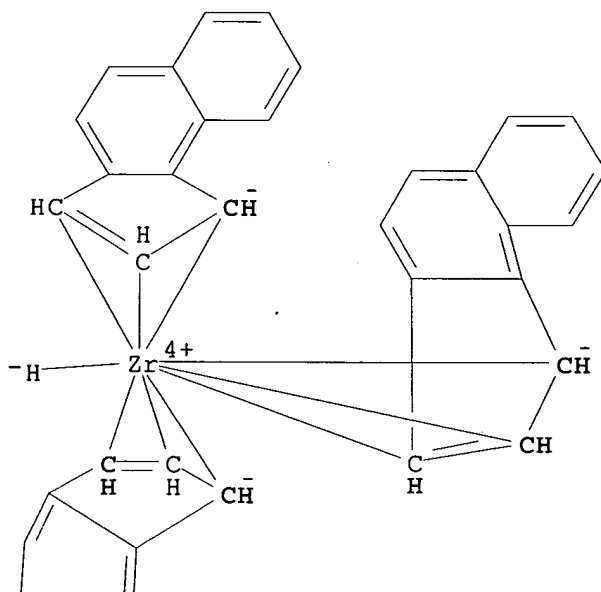
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

(polymn. catalyst; manuf. of branched ethylene polymers with improved moldability and mech. strength)

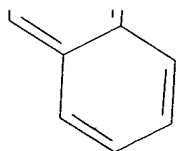
RN 683752-59-2 HCAPLUS

CN Zirconium, tris[(1,2,3- η)-1H-benz[e]inden-1-yl]hydro- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



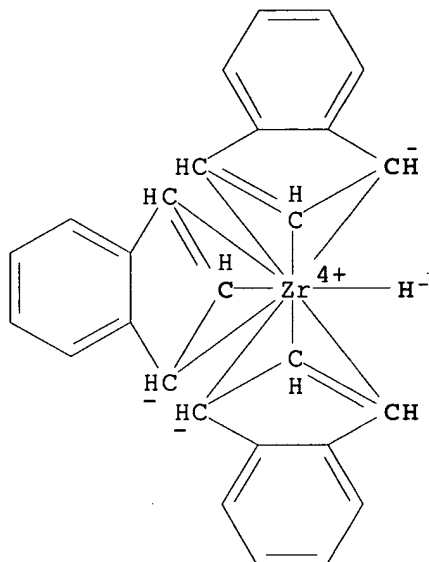
IT 683752-55-8P

RL: CAT (Catalyst use); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(polymn. catalyst; manuf. of branched ethylene polymers with improved moldability and mech. strength)

RN 683752-55-8 HCAPLUS

CN Zirconium, hydrotris[(1,2,3- η)-1H-inden-1-yl]- (9CI) (CA INDEX NAME)



CC 37-3 (Plastics Manufacture and Processing)

Section cross-reference(s): 29, 35

IT 683752-59-2P

RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

(polymn. catalyst; manuf. of branched ethylene polymers with improved moldability and mech. strength)

IT 683752-55-8P

RL: CAT (Catalyst use); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(polymn. catalyst; manuf. of branched ethylene polymers with improved moldability and mech. strength)

L30 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN

2004:370945 Document No. 140:375680 Novel transition metal compound, catalyst for olefin polymerization and method for producing polyolefin. Seki, Takashi; Shimizu, Hiroyuku; Takahashi, Tamotsu; Nakajima, Kiyohiko; Fukuda, Tetsuro (Japan Polyethylene Corporation, Japan). PCT Int. Appl. WO 2004037841 A1 20040506, 73 pp. DESIGNATED STATES: W: DE, US. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2003-JP13610 20031024. PRIORITY: JP 2002-311451 20021025.

AB The present invention relates to a novel transition metal compd. wherein the transition metal belongs to Group IV of the Periodic Table and the transition metal compd. has a hydrogen atom ligand and

The current Application

three cyclopentadienyl ligands comprising ≥ 1 substituted cyclopentadienyl ligand. The novel transition metal compd. can be used as a component of a catalyst exhibiting high activity for olefin polymn. and is characteristic in contg. no halogen element. Thus, 1 mmol bisindenylzirconium dichloride and 2 mmol butyllithium were stirred, 4 mmol indene was added therein and reacted to give trisindenylzirconium hydride with yield 64%, 5.0 μmol of which was mixed with 5.0 mmol Me aluminoxane and used for a polymn. of ethylene, showing polymn. activity 74 kg/mmol Zr \cdot Mpa \cdot hour, Mw 102,600, and polydispersity 2.97.

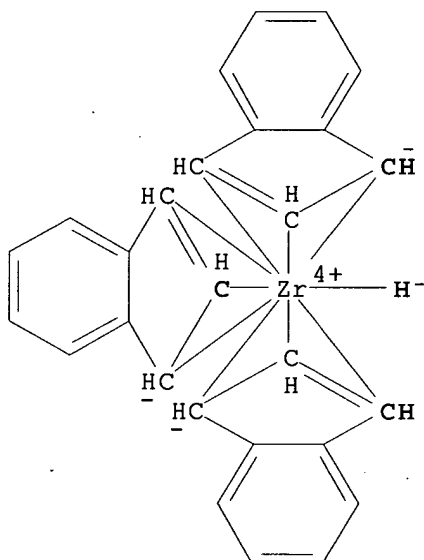
IT 683752-55-8P

RL: CAT (Catalyst use); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(polymn. catalyst, optionally intermediate; prepn. of transition metal compds. for olefin polymn.)

RN 683752-55-8 HCAPLUS

CN Zirconium, hydrotris[(1,2,3- η)-1H-inden-1-yl]- (9CI) (CA INDEX NAME)



IT 683752-56-9P 683752-57-0P 683752-58-1P

683752-59-2P 683752-60-5P 683771-52-0P

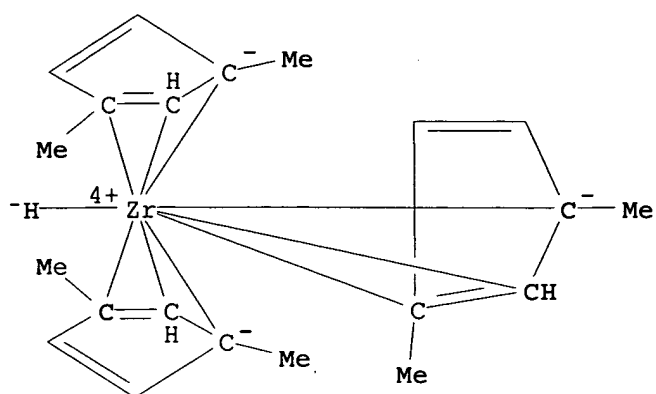
683771-53-1P 683771-54-2P

RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

(polymn. catalyst; prepn. of transition metal compds. for olefin polymn.)

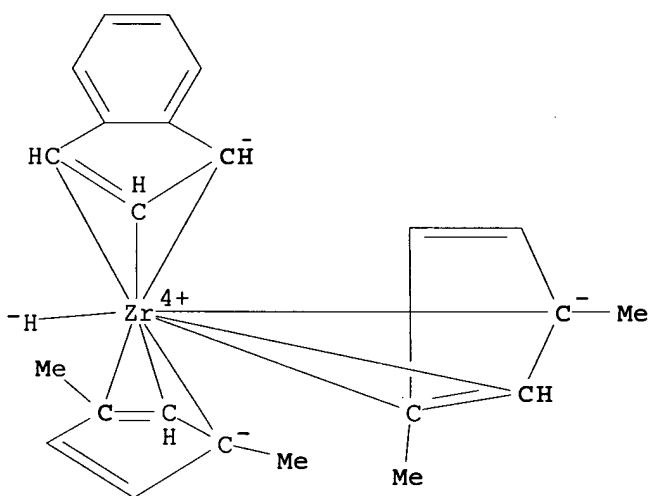
RN 683752-56-9 HCAPLUS

CN Zirconium, tris[(1,2,3- η)-1,3-dimethyl-2,4-cyclopentadien-1-yl]hydro- (9CI) (CA INDEX NAME)



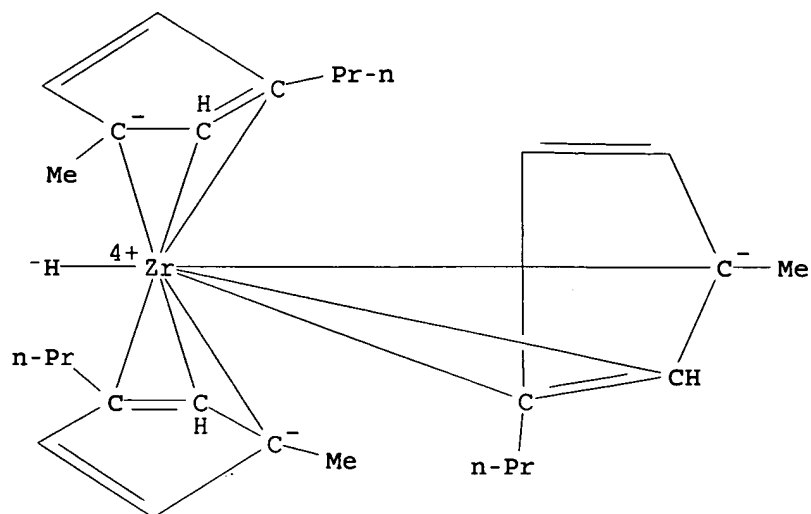
RN 683752-57-0 HCAPLUS

CN Zirconium, bis[(1,2,3- η)-1,3-dimethyl-2,4-cyclopentadien-1-yl]hydro[(1,2,3- η)-1H-inden-1-yl]- (9CI) (CA INDEX NAME)



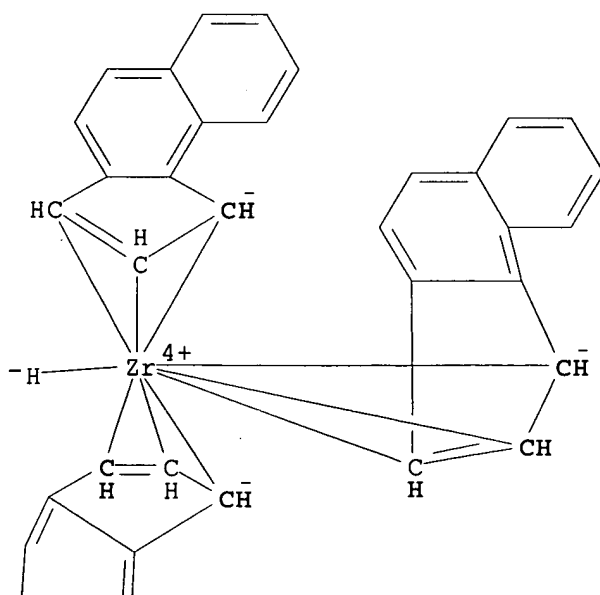
RN 683752-58-1 HCAPLUS

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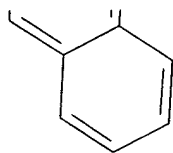


RN 683752-59-2 HCAPLUS
 CN Zirconium, tris[(1,2,3-η)-1H-benz[e]inden-1-yl]hydro- (9CI) (CA
 INDEX NAME)

PAGE 1-A

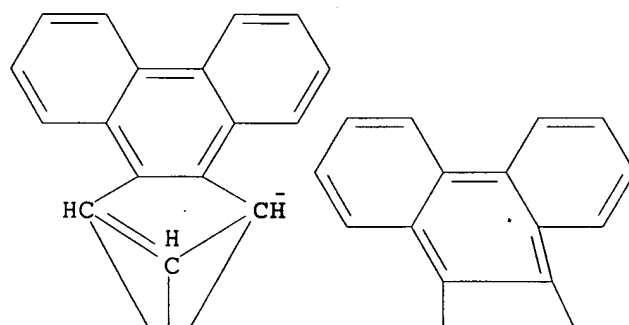


PAGE 2-A

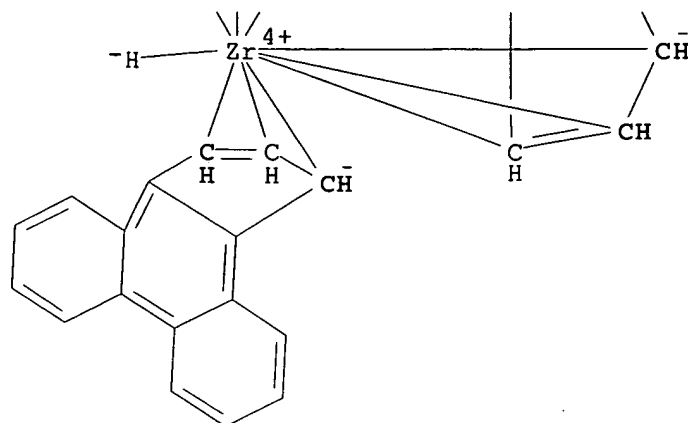


RN 683752-60-5 HCAPLUS
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 (9CI) (CA INDEX NAME)

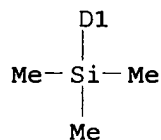
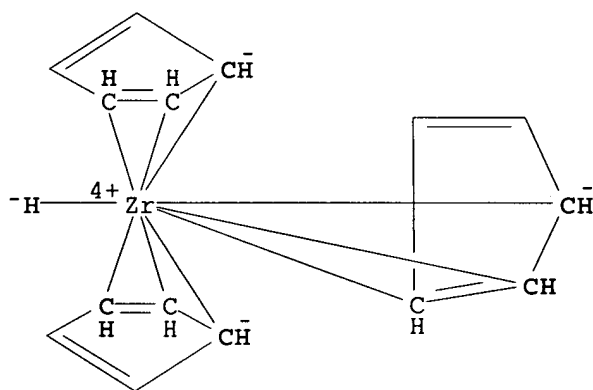
PAGE 1-A



PAGE 2-A

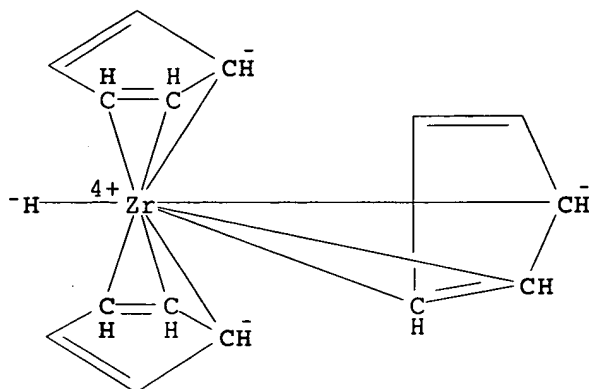


RN 683771-52-0 HCAPLUS
 CN Zirconium, bis[(1,2,3- η)-2,4-cyclopentadien-1-yl]hydro[(1,2,3- η)-(trimethylsilyl)-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)

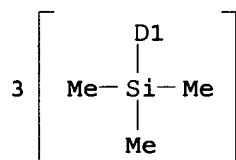


RN 683771-53-1 HCAPLUS
 CN Zirconium, hydrotris[(1,2,3- η)-(trimethylsilyl)-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)

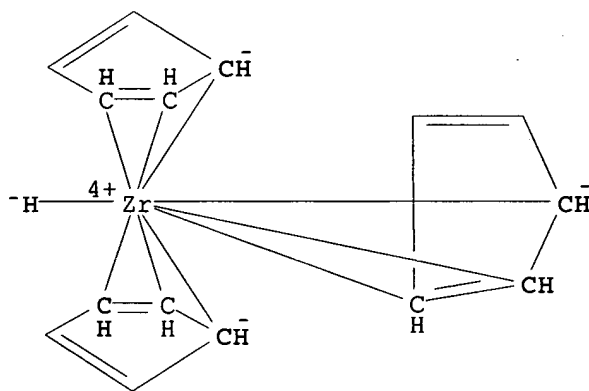
PAGE 1-A



PAGE 2-A



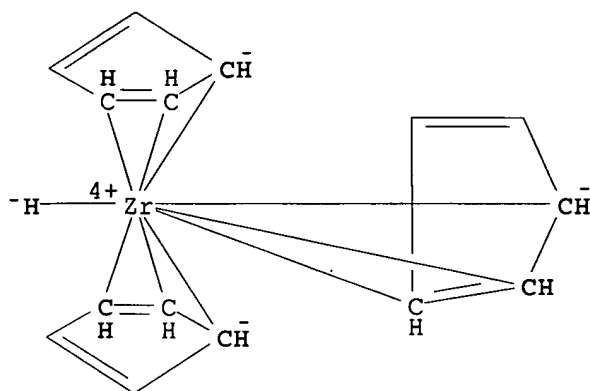
RN 683771-54-2 HCAPLUS
 CN Zirconium, hydrotris[(1,2,3-η)-methyl-2,4-cyclopentadien-1-yl]-(9CI) (CA INDEX NAME)



3 (D1-Me)

IT 683771-51-9P
 RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
 (prepn. of transition metal compds. for olefin polymn.)
 RN 683771-51-9 HCAPLUS

CN Zirconium, bis[(1,2,3- η)-2,4-cyclopentadien-1-yl]hydro[(1,2,3- η)-methyl-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)



D1-Me

IC ICM C07F017-00
ICS C07F007-00; C07F007-08; C08F004-646
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 67
IT **683752-55-8P**
RL: CAT (Catalyst use); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(polymn. catalyst, optionally intermediate; prepn. of transition metal compds. for olefin polymn.)
IT **683752-56-9P 683752-57-0P 683752-58-1P**
683752-59-2P 683752-60-5P 683771-52-0P
683771-53-1P 683771-54-2P
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(polymn. catalyst; prepn. of transition metal compds. for olefin polymn.)
IT **683771-51-9P**
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(prepn. of transition metal compds. for olefin polymn.)

=> d l31 cbib abs hitstr hitind 1-75

L31 ANSWER 1 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
2002:710141 Document No. 139:7211 Synthesis of hetero-bimetallic metallocene complexes and their catalytic activities for ethylene polymerization. Huang, Jiling; Feng, Zuofeng; Wang, Hong; Qian, Yanlong; Sun, Junquan; Xu, Yongjin; Chen, Wei; Zheng, Gang (Laboratory of Organometallic Chemistry, East China University of Science and Technology, Shanghai, 200237, Peop. Rep. China). Journal of Molecular Catalysis A: Chemical, 189(2), 187-194 (English) 2002. CODEN: JMCCF2. ISSN: 1381-1169. Publisher: Elsevier Science B.V..

AB Five new hetero-bimetallic metallocene complexes were synthesized by

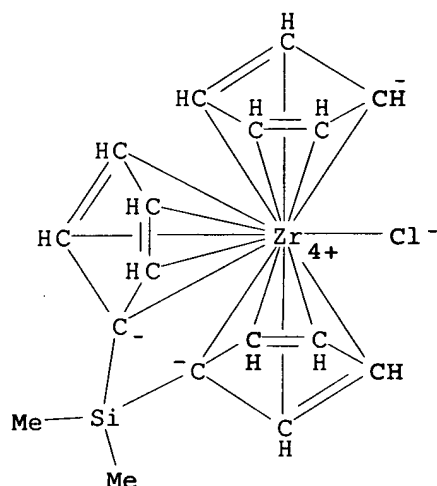
the reaction of RCpTiCl_3 and a Si-bridged zirconocene complex in refluxing toluene. They were all well characterized. These complexes activated with methylaluminoxane (MAO) are highly active catalysts for the polymn. of ethylene. The mol. wt. ($M_w = 28,957\text{--}124,089$) and the mol. wt. distribution ($MWD = 2.04\text{--}3.01$) of the polymer generated from the bimetallic catalytic system were higher than that obtained by Cp_2ZrCl_2 .

IT 179400-07-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (prepn. of hetero-bimetallic metallocene complexes and their
 catalytic activities for ethylene polymn.)

RN 179400-07-8 HCAPLUS

CN Zirconium, chloro($\eta^5\text{-2,4-cyclopentadien-1-yl}$)[(dimethylsilylene)bis($\eta^5\text{-2,4-cyclopentadien-1-ylidene}$)]-(9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 29

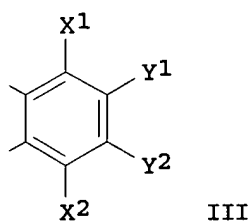
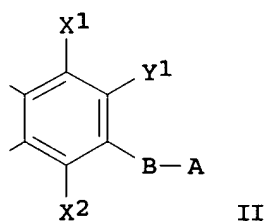
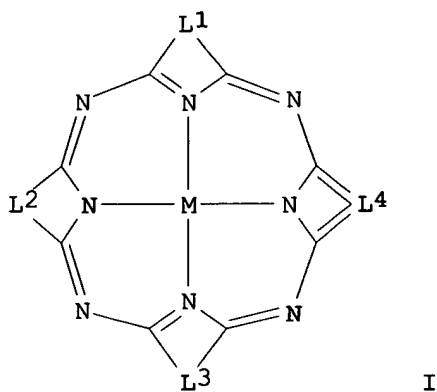
IT 179400-07-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (prepn. of hetero-bimetallic metallocene complexes and their
 catalytic activities for ethylene polymn.)

L31 ANSWER 2 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

2002:503747 Document No. 137:86006 Phthalocyanines and their use in recording layers of optical recording media. Kiyono, Kazuhiro; Nakagawa, Shinichi; Misawa, Tsutayoshi (Mitsui Chemicals Inc., Japan; Yamamoto Chemicals Inc.). Jpn. Kokai Tokkyo Koho JP 2002188019 A2 20020705, 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2000-386989 20001220.

GI



AB The phthalocyanines are shown as I [M = two H, divalent metal, tri- or tetravalent substituted metal, oxymetal; L1-L4 = II, III; at least one of L1-L4 = II; X1, X2 = (un)substituted C1-10 linear or branched alkyl(thio), (un)substituted C1-15 linear or branched alkoxy; Y1, Y2 = H, NO₂, halo; A = metal compd. residue; B = group for linking phthalocyanines and A]. The media, e.g., write-once read-many disk of CD-R (CD-recordable), show high sensitivity in high-speed high-d. recording and improved jitter and deviation characteristics.

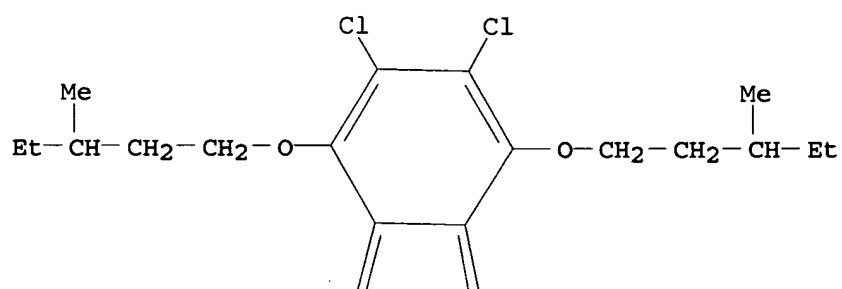
IT 440364-90-9 440364-92-1

RL: TEM (Technical or engineered material use); USES (Uses)
(phthalocyanines and their use in recording layers of optical recording media)

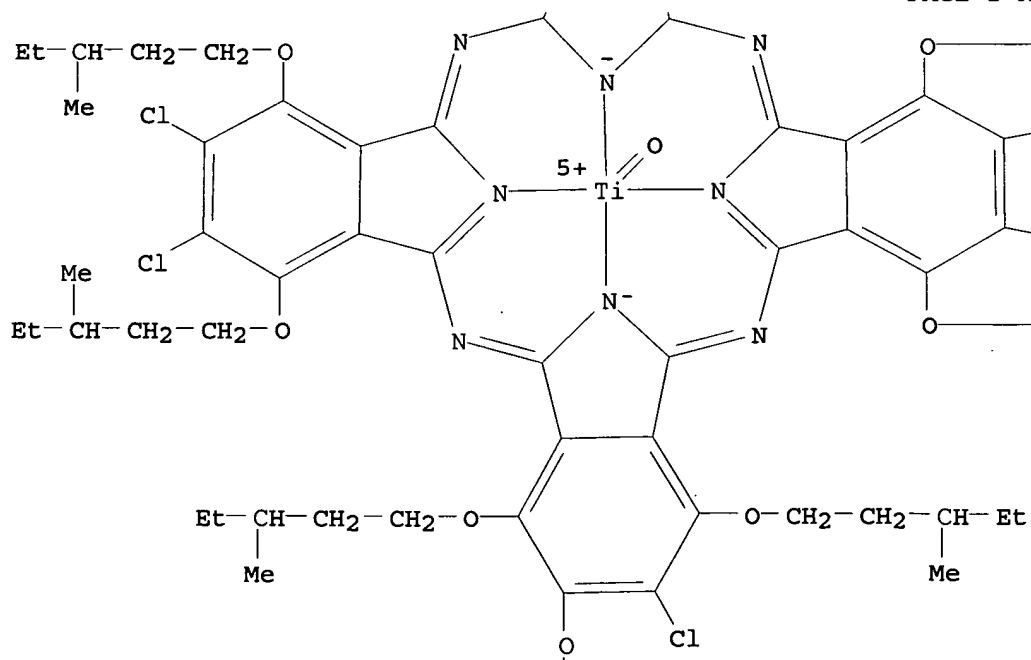
RN 440364-90-9 HCAPLUS

CN Scandium, bis(η⁵-2,4-cyclopentadien-1-yl) [μ-[(1,2,3,4,5-η)-[3-[[3,9,10,16,17,23,24-heptachloro-1,4,8,11,15,18,22,25-octakis[(3-methylpentyl)oxy]-29H,31H-phthalocyanin-2-yl-κN29,κN30,κN31,κN32]oxy]phenyl]methyl 2,4-cyclopentadiene-1-carboxylato(3-)] (oxotitanium) - (9CI) (CA INDEX NAME)

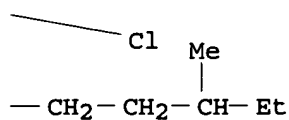
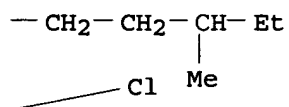
PAGE 1-A



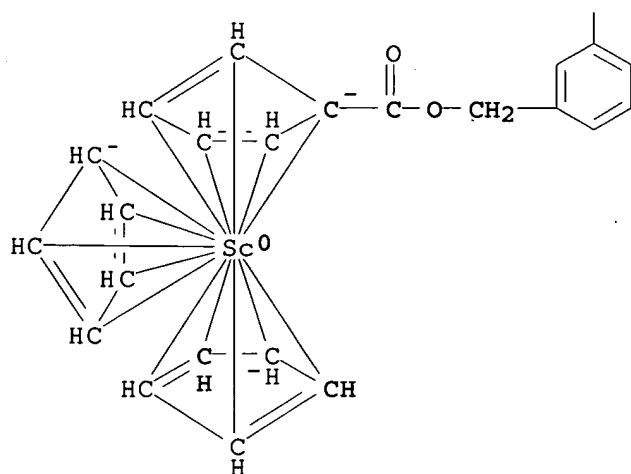
PAGE 2-A



PAGE 2-B

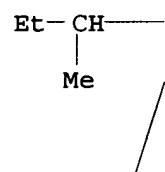
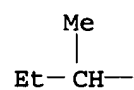


PAGE 3-A

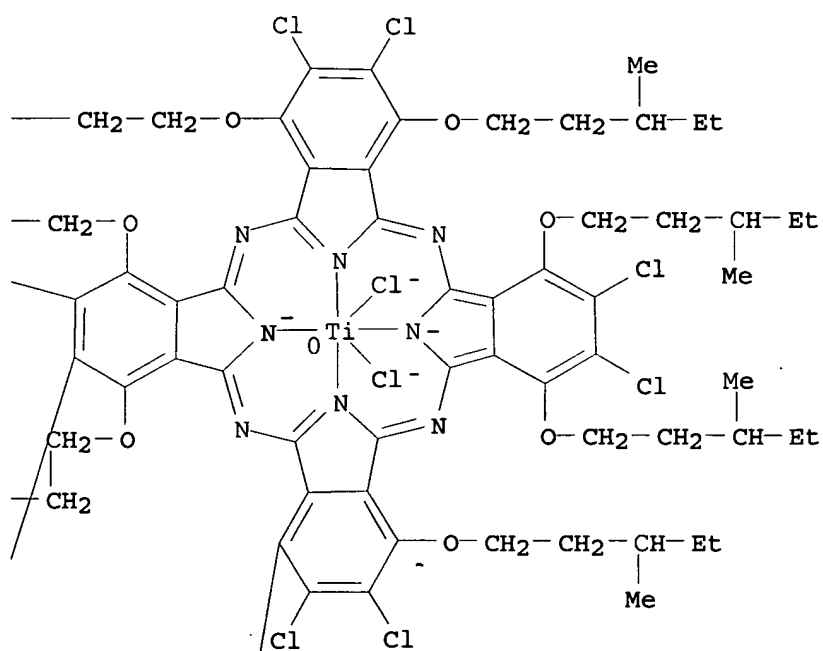


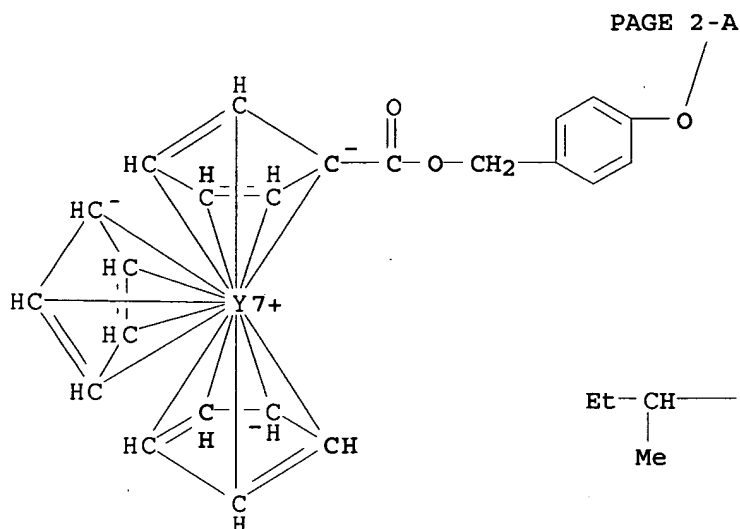
RN 440364-92-1 HCAPLUS
 CN Yttrium, bis(η⁵-2,4-cyclopentadien-1-yl) (dichlorotitanium) [μ-
 [(1,2,3,4,5-η) - [4- [[3,9,10,16,17,23,24-heptachloro-
 1,4,8,11,15,18,22,25-octakis[(3-methylpentyl)oxy]-29H,31H-
 phthalocyanin-2-yl-κN29,κN30,κN31,κN32]oxy]p
 henyl]methyl 2,4-cyclopentadiene-1-carboxylato(3-)] - (9CI) (CA
 INDEX NAME)

PAGE 1-A

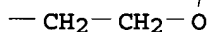


PAGE 1-B





PAGE 2-B



IC ICM C09B047-18
ICS B41M005-26; G11B007-24; C07F015-00; C07F015-02; C07F017-02
CC 74-12 (Radiation Chemistry, Photochemistry, and Photographic and
Other Reprographic Processes)
Section cross-reference(s): 28, 29, 47
IT 440364-77-2 440364-79-4 440364-81-8 440364-83-0 440364-85-2
440364-87-4 **440364-90-9 440364-92-1**
440364-94-3 440366-90-5 440366-91-6 440366-93-8
RL: TEM (Technical or engineered material use); USES (Uses)
(phthalocyanines and their use in recording layers of optical
recording media)

L31 ANSWER 3 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
2001:759757 Document No. 136:279719 Bis(η⁵-
cyclopentadienyl)bistriphenylsilanolatozirconium(IV): a new
precursor for ethylene polymerization catalysis. Altomare,
Angelina; Candian, Roberta; Michelotti, Marco; Pampaloni, Guido;
Ciardelli, Francesco (Dipartimento Chimica, Chimica Industriale,
Pisa, 56126, Italy). e-Polymers [online computer file] No pp.

given, Paper No. 8 (English) 2001. CODEN: EPOLCI. URL:
http://www.e-polymers.org/papers/altomare_260701.pdf Publisher:
 European Polymer Federation.

AB Trialkylsilanols were reported to modify and also to improve the catalytic performance in ethylene polymn. when added to zirconocene/methyl-aluminoxane (MAO) systems. In order to obtain more information about the chem. involved, a new stable catalytic precursor was investigated in this work. The precursor bis(η^5 -cyclopentadienyl)bistriphenylsilanolatozirconium(IV) [ZrCp₂(OSiPh₃)₂] was compared to ZrCp₂(CH₃)₂ and ZrCp₄, which can generate ZrCp₂(OSiPh₃)₂ in situ on triphenylsilanol addn. In ethylene polymn., ZrCp₂(OSiPh₃)₂ exhibits a comparable activity and a larger stability than dicyclopentadienylzirconium complexes. On addn. of triphenylsilanol to zirconocenes, the productivity increased and the mol. wt. sharply decreased, thus suggesting the occurrence of ligand substitution in soln. The reported results are discussed with ref. to the proposed mechanism of ethylene polymn. with the conventional ZrCp₂Cl₂/MAO system.

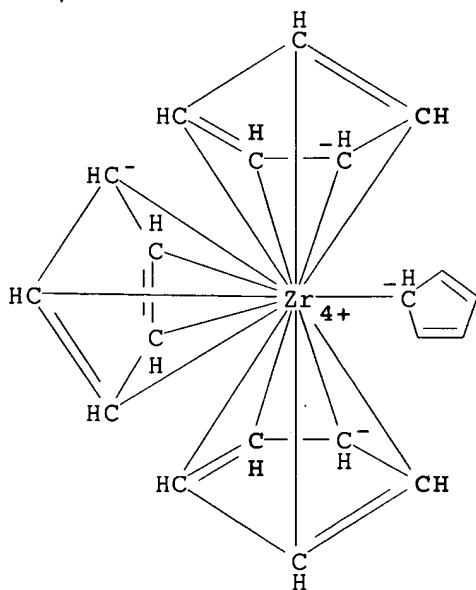
IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium

RL: CAT (Catalyst use); USES (Uses)

(bis(η^5 -cyclopentadienyl)bistriphenylsilanolatozirconium(IV)
 as a precursor for ethylene polymn. catalysis)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

IT 75-24-1, Trimethylaluminum 791-31-1, Triphenylsilanol

1273-01-4, Tetrakis(cyclopentadienyl)zirconium 1291-32-3,
 Zirconocene dichloride 105472-97-7

RL: CAT (Catalyst use); USES (Uses)

(bis(η^5 -cyclopentadienyl)bistriphenylsilanolatozirconium(IV)
 as a precursor for ethylene polymn. catalysis)

L31 ANSWER 4 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

2001:260623 Document No. 135:46265 Synthesis and Structural Behavior

of the Tris(η -cyclopentadienyl)zirconium-Betaine Complex
 $\text{Cp}_2[\eta^5\text{-C}_5\text{H}_4\text{B}(\text{C}_6\text{F}_5)_3]\text{Zr}$. Kleigrew, Nina; Brackemeyer, Thomas;
 Kehr, Gerald; Froehlich, Roland; Erker, Gerhard (Organisch-
 Chemisches Institut, Universitaet Muenster, Muenster, D-48149,
 Germany). Organometallics, 20(10), 1952-1955 (English) 2001
 . CODEN: ORGND7. ISSN: 0276-7333. OTHER SOURCES: CASREACT
 135:46265. Publisher: American Chemical Society.

AB Treatment of the reagent $[\text{C}_5\text{H}_4\text{B}(\text{C}_6\text{F}_5)_3]\text{Na}\cdot\text{Li}\cdot\text{Et}_2\text{O}$ (4) with
 zirconocene dichloride gave the neutral tris(cyclopentadienyl)Zr-
 betaine-type complex $(\eta^5\text{-Cp})_2[\eta^5\text{-C}_5\text{H}_4\text{B}(\text{C}_6\text{F}_5)_3]\text{Zr}$ (1). In
 the crystal complex 1 contains the three η -cyclopentadienide
 ligands in a nearly trigonal-planar coordination around Zr with a
 pronounced Zr-F-C(aryl) coordination perpendicular to it. The Zr-F
 bond length is 2.310(3) Å. The Zr-F-C(aryl) coordination is
 persistent in soln. The activation energy of the reversible
 cleavage of the Zr-F linkage of 1 was detd. as $\Delta G_{\text{thermod.}}(\text{Zr-}$
 $\text{F})_{\text{diss}}(253\text{ K}) = 10.2 \pm 0.2\text{ kcal mol}^{-1}$ by dynamic ^{19}F NMR
 spectroscopy in toluene- d_8 .

IT 344899-51-0P

RL: PEP (Physical, engineering or chemical process); PRP
 (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC
 (Process)

(prep., crystal structure and fluxionality of)

RN 344899-51-0 HCAPLUS

CN Zirconium, [bis(pentafluorophenyl)boron]bis(η^5 -2,4-
 cyclopentadien-1-yl) [μ -(η^5 -2,4-cyclopentadien-1-
 ylidene)] [μ -[2-(fluoro- κ F)-3,4,5,6-tetrafluorophenyl-
 κ C]]-, compd. with dichloromethane (1:1) (9CI) (CA INDEX
 NAME)

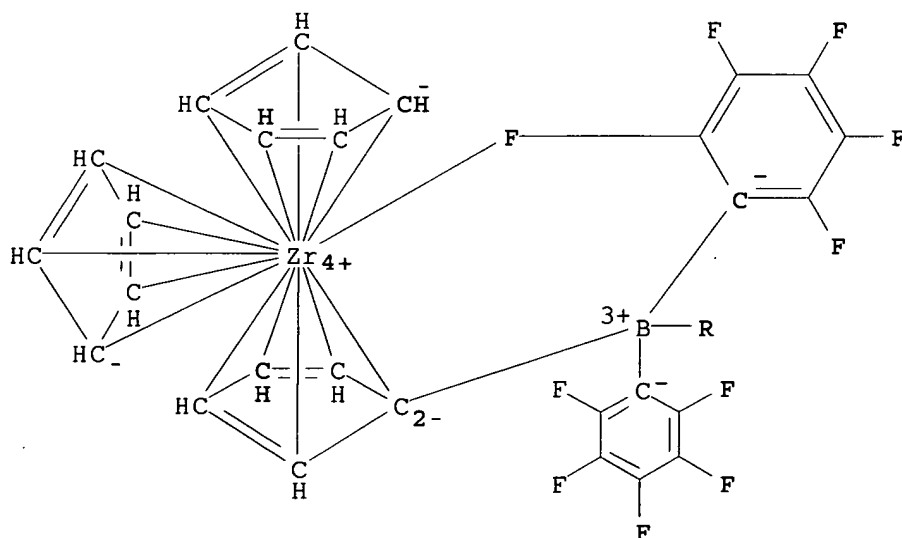
CM 1

CRN 344899-50-9

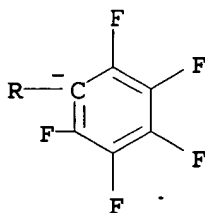
CMF C33 H14 B F15 Zr

CCI CCS

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PAGE 2-A



CM 2

CRN 75-09-2
CMF C H2 Cl2

Cl-CH₂-Cl

CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75

IT 344899-51-0P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(prepn., crystal structure and fluxionality of)

L31 ANSWER 5 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

2000:491192 Document No. 133:222793 Coordination chemistry of {[Zr]-Cl-[Zr]}⁺ complexes. Jacobsen, Heiko; Brackemeyer, Thomas; Berke, Heinz; Erker, Gerhard; Frohlich, Roland (Anorganisch-chemisches Institut, Universitat Zurich-Irchel, Zurich, CH-8057, Switz.). European Journal of Inorganic Chemistry (7), 1423-1428 (English) 2000. CODEN: EJICFO. ISSN: 1434-1948. Publisher: Wiley-VCH Verlag GmbH.

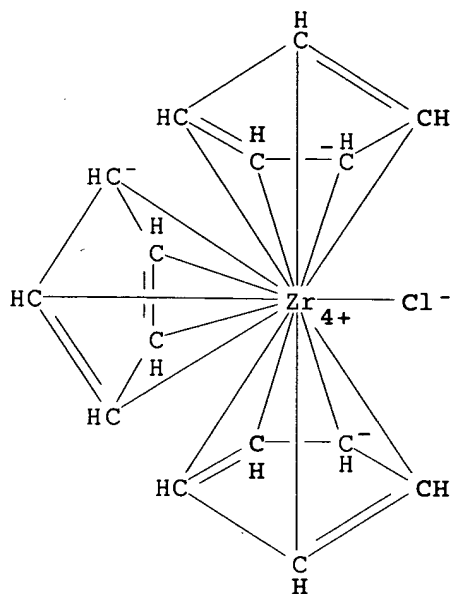
AB Treatment of the tris(cyclopentadienyl)zirconium cation (1⁺) with zirconocene dichloride gave, in almost quant. yield, the 1:1 adduct 7⁺, which was isolated with [(CH₃)B(C₆F₅)₃]⁻ as the counterion. Reaction of 1⁺ with the organometallic ligand Cp₃ZrCl afforded the 1:1 adduct 8⁺, again isolated with [(CH₃)B(C₆F₅)₃]⁻. The x-ray anal. revealed that 7⁺ displays a strongly bent Zr-Cl-Zr coordination mode, in contrast to 8⁺, which has a tendency to linear coordination. A theor. anal. suggests that a subtle balance between steric and electronic factors detts. the geometries in such organometallic adducts.

IT 62343-37-7

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(optimized structure and reaction with
tris(cyclopentadienyl)methylzirconium in presence of
tris(pentafluorophenyl)borane)

RN 62343-37-7 HCAPLUS

CN Zirconium, chlorotris(η⁵-2,4-cyclopentadien-1-yl)- (9CI) (CA
INDEX NAME)

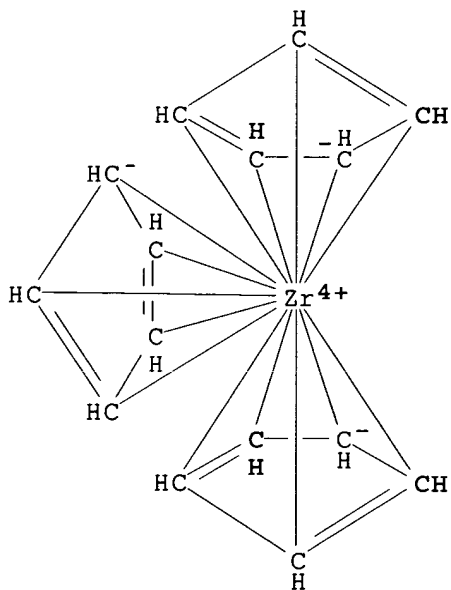


IT 185549-25-1

RL: PRP (Properties)
(optimized structures for)

RN 185549-25-1 HCAPLUS

CN Zirconium(1+), tris(η5-2,4-cyclopentadien-1-yl) - (9CI) (CA
INDEX NAME)



IT 291546-02-6P 291546-04-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)

(prepn. and crystal structure of)

RN 291546-02-6 HCAPLUS

CN Zirconium(1+), μ-chlorochloropentakis(η5-2,4-cyclopentadien-1-

yl)di-, (T-4)-methyltris(pentafluorophenyl)borate(1-), compd. with
dichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 75-09-2
CMF C H2 Cl2

Cl-CH₂-Cl

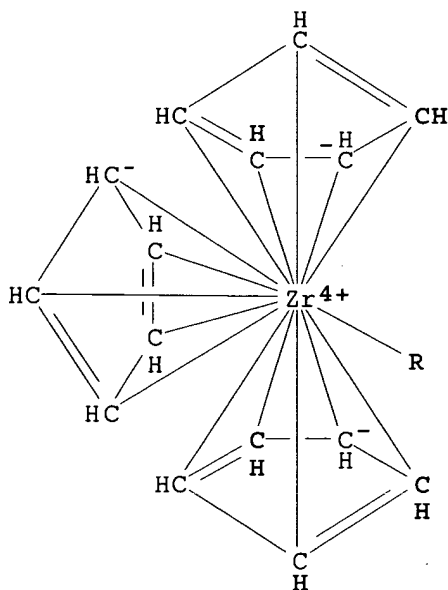
CM 2

CRN 291546-01-5
CMF C25 H25 Cl2 Zr2 . C19 H3 B F15

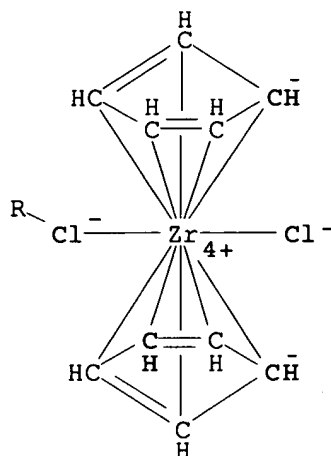
CM 3

CRN 291546-00-4
CMF C25 H25 Cl2 Zr2
CCI CCS

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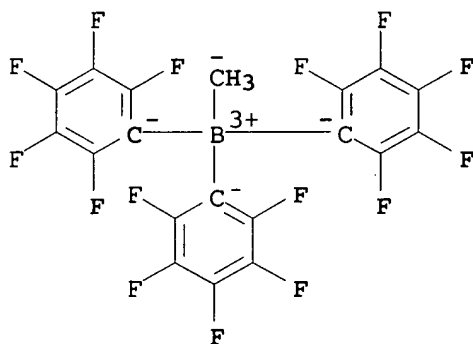


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CM 4

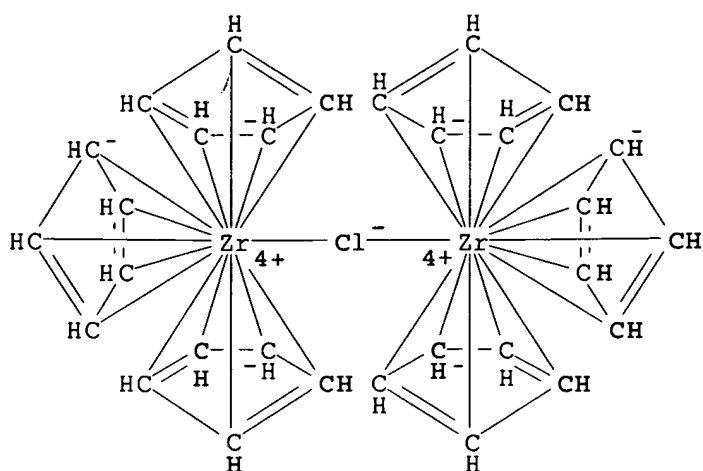
CRN 133445-48-4
 CMF C19 H3 B F15
 CCI CCS



RN 291546-04-8 HCAPLUS
 CN Zirconium(1+), μ -chlorohexakis(η^5 -2,4-cyclopentadien-1-yl)di-
 , (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX
 NAME)

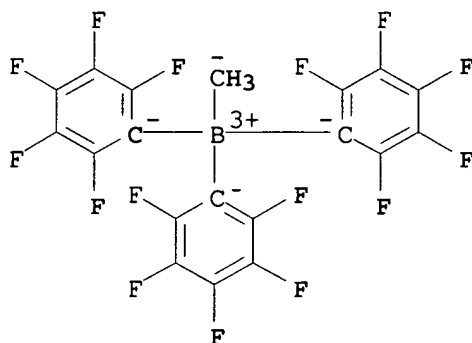
CM 1

CRN 291546-03-7
 CMF C30 H30 Cl Zr2
 CCI CCS



CM 2

CRN 133445-48-4
 CMF C19 H3 B F15
 CCI CCS



IT 291546-01-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP
 (Preparation)
 (prepn. and mol. structure of)

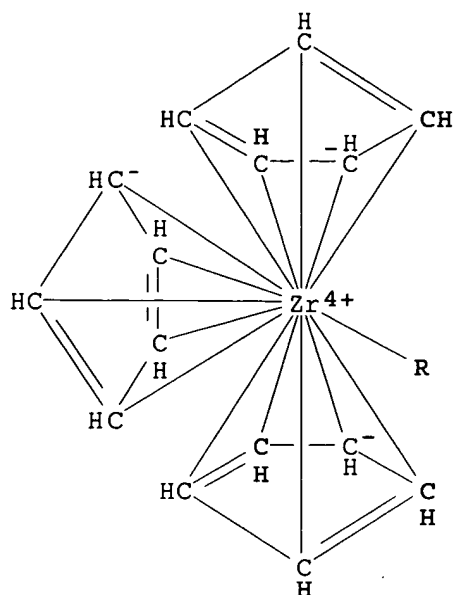
RN 291546-01-5 HCAPLUS

CN Zirconium(1+), μ -chlorochloropentakis(η^5 -2,4-cyclopentadien-1-yl)di-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA
 INDEX NAME)

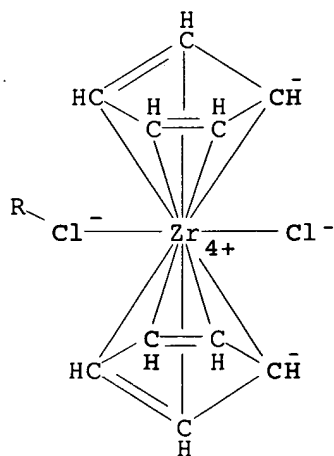
CM 1

CRN 291546-00-4
 CMF C25 H25 Cl2 Zr2
 CCI CCS

PAGE 1-A

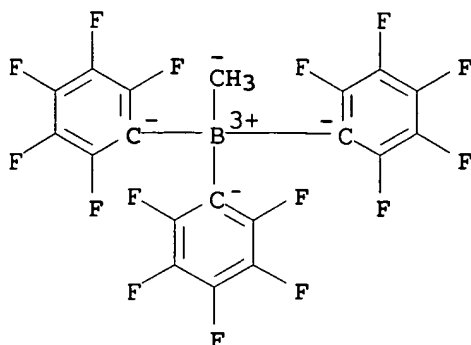


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CM 2

CRN 133445-48-4
CMF C19 H3 B F15
CCI CCS

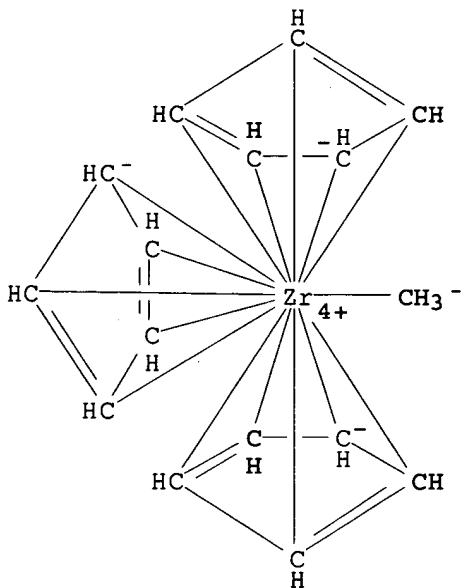


IT 185549-24-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with cyclopentadienylzirconium chloride in presence of
tris(pentafluorophenyl)borane)

RN 185549-24-0 HCAPLUS

CN Zirconium, tris(η5-2,4-cyclopentadien-1-yl)methyl- (9CI) (CA
INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 75

IT 1291-32-3 62343-37-7

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(optimized structure and reaction with
tris(cyclopentadienyl)methylzirconium in presence of
tris(pentafluorophenyl)borane)

IT 185549-25-1

RL: PRP (Properties)
(optimized structures for)

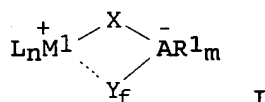
IT 291546-02-6P 291546-04-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)

- (prepn. and crystal structure of)
- IT 291546-01-5P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and mol. structure of)
- IT 185549-24-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction with cyclopentadienylzirconium chloride in presence of tris(pentafluorophenyl)borane)

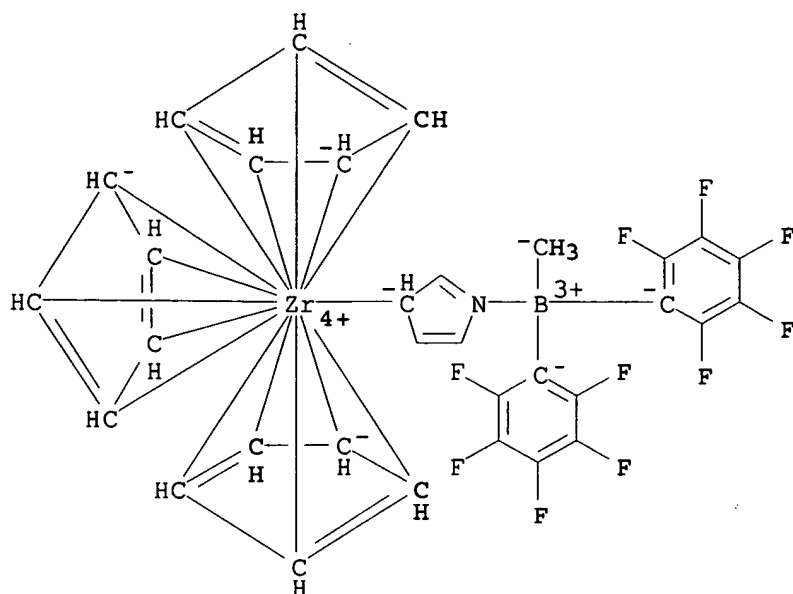
L31 ANSWER 6 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
 2000:421191 Document No. 133:59217 Zwitterionic, neutral transition metal compounds containing boron for polymerization of olefins.
 Erker, Gerhard; Kehr, Gerald; Schottek, Jorg; Kratzer, Roland
 (Targor GmbH, Germany). PCT Int. Appl. WO 2000035973 A1
 20000622, 108 pp. DESIGNATED STATES: W: BR, JP, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (German). CODEN: PIXXD2. APPLICATION: WO 1999-EP9682
 19991209. PRIORITY: DE 1998-19857377 19981212; DE 1999-19903306 19990128.

GI



- AB The invention relates to a zwitterionic, neutral transition metal compd. I [L = π -ligand or electron donor, n = 1-4, M = Group IIb, IVb, Vb, or VIb metal, X = heteroatom, (non)arom. heterocyclic group, or C1-40 hydrocarbon group, Y, R1 = (halogenated) C1-40 hydrocarbon group, f = 0 or 1, A = Group Ib, IIb, IIIa, IVa, VIb, VIIb, or VIIIb metal atom (preferably B), m = 1-5] which can be advantageously used for the polymn. of olefins. As a result, the use of aluminoxanes such as methylaluminoxane (MAO) as a co-catalyst can be foregone, and yet a high catalyst activity and favorable polymer morphol. can be achieved. A typical I was manufd. by mixing 0.133 g bis(η 5-cyclopentadienyl)dimethylzirconium with 0.217 g bis(pentafluorophenyl)pyrrolylborane 5 min in 10 mL PhMe.

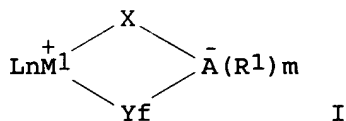
- IT 261347-75-5P
 RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
 (zwitterionic, neutral transition metal compds. contg. boron for polymn. of olefins)
- RN 261347-75-5 HCAPLUS
 CN Zirconium, tris(η 5-2,4-cyclopentadien-1-yl) [methylbis(pentafluorophenyl)boron] [μ -(3H-pyrrol-3-yl)- κ C: κ N)]- (9CI) (CA INDEX NAME)



IC ICM C08F110-02
ICS C08F004-643
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 67, 78
IT 261347-75-5P 261347-76-6P 261376-52-7P
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP
(Preparation); USES (Uses)
(zwitterionic, neutral transition metal compds. contg. boron for
polymn. of olefins)

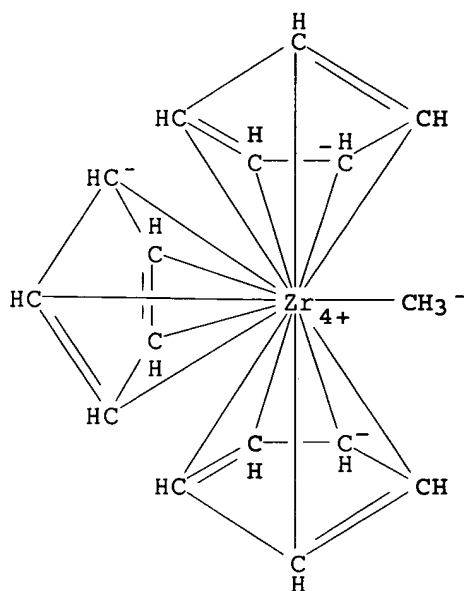
L31 ANSWER 7 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
2000:396574 Document No. 133:43967 Neutral zwitterionic transition
metal compounds for polymerization of olefins. Erker, Gerhard;
Kehr, Gerald; Schottek, Joerg; Kratzer, Roland (Targor G.m.b.H.,
Germany). Ger. Offen. DE 19857377 A1 20000615, 40 pp.
(German). CODEN: GWXXBX. APPLICATION: DE 1998-19857377 19981212.

GI

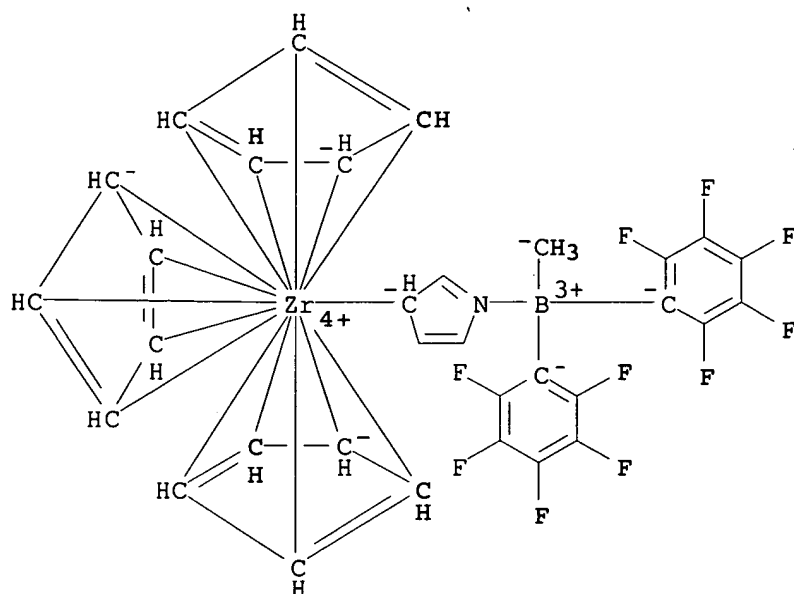


AB The metal complexes I [A = Group IB, IIB, IIIA-VA, VIB-VIIIB
element; each L = π -bonded ligand, electron donor; M1 = Group
IIIB-VIB metal; R1, Y = C1-40 (halo)hydrocarbyl; X = hetero atom,
heterocyclic residue, C1-40 hydrocarbylene; f = 0, 1; m = 1-5; n =
1-4] show a high catalyst activity and provide a good polymer
morphol. without the use of aluminoxanes as cocatalysts. Thus,
reaction of (C6F5)2BF.OEt2 with pyrrolyllithium gave (C6F5)2BR (R =
pyrrolyl) (II). Reaction of Cp2ZrMe2 (Cp = η^5 -cyclopentadienyl)
with II gave a I, which, after treatment with iso-Bu3Al, polymd.
ethylene at 25°/10 bars with an activity of 0.75 kg polymer/g

metallocene per h.
 IT 185549-24-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (neutral zwitterionic transition metal compds. for polymn. of
 olefins)
 RN 185549-24-0 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)methyl- (9CI) (CA
 INDEX NAME)



IT 261347-75-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (neutral zwitterionic transition metal compds. for polymn. of
 olefins)
 RN 261347-75-5 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl) [methylbis(pentafluorophenyl)boron] [μ -(3H-pyrrol-3-yl- κ C: κ N)]- (9CI) (CA INDEX NAME)



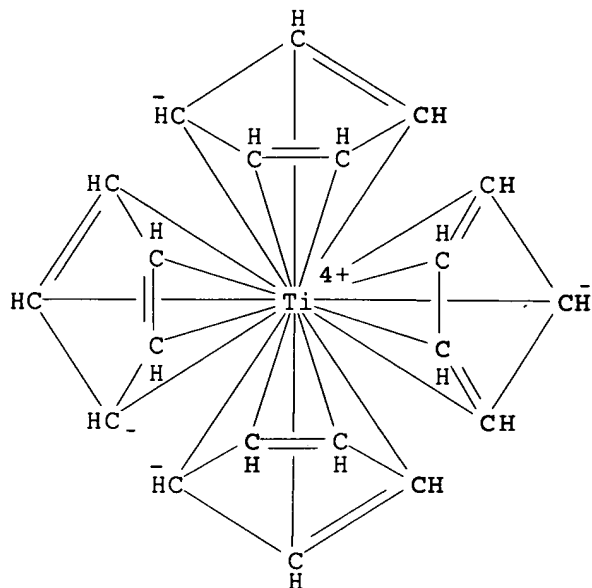
- IC ICM C07F017-00
ICS C08F004-64; C08F010-00
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29
IT 12636-72-5, Bis(cyclopentadienyl)dimethylzirconium 20671-52-7,
Pyrrolyllithium 75374-50-4 185549-24-0 197009-46-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(neutral zwitterionic transition metal compds. for polymn. of
olefins)
IT 261347-75-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(neutral zwitterionic transition metal compds. for polymn. of
olefins)

L31 ANSWER 8 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
2000:113709 Document No. 132:194442 Carbon monoxide and tertiary
phosphines as ligands in cyclopentadienyl derivatives of Group 4
elements in high oxidation state. Pampaloni, Guido; Tripepi,
Giovanna (Dipartimento di Chimica e Chimica Industriale, Universita
di Pisa, Pisa, I-56126, Italy). Journal of Organometallic
Chemistry, 593-594, 19-26 (English) 2000. CODEN: JORCAI.
ISSN: 0022-328X. OTHER SOURCES: CASREACT 132:194442. Publisher:
Elsevier Science S.A..

- AB The titanocene dicarbonyl dication $[\text{TiCp}_2(\text{CO})_2][\text{BPh}_4]_2$, (1) has been
obtained in toluene under carbon monoxide by double protonation of
 TiCp_4 with $[\text{NHnBu}_3][\text{BPh}_4]$ or by two-electron oxidn. of $\text{TiCp}_2(\text{CO})_2$
with $[\text{FeCp}_2][\text{BPh}_4]$. Protonation reactions on ZrCp_4 and HfCp_4
proceed with elimination of 1 mol of cyclopentadiene independently
on the ammonium salt/ MCp_4 molar ratio used. By this route the high
electrophilic, solvent-free $[\text{ZrCp}_3]^+$ cation has been isolated and
characterized by IR, $^1\text{H-NMR}$ and elemental anal. In the case of
hafnium, the isolation has not been possible; nevertheless, in the
presence of CO a rare example of a carbonyl deriv. of hafnium(IV),
 $[\text{HfCp}_3(\text{CO})][\text{BPh}_4]$, has been isolated and characterized.
IT 11079-32-6, Tetrakis(cyclopentadienyl)titanium
RL: RCT (Reactant); RACT (Reactant or reagent)

(double protonation of)

RN 11079-32-6 HCAPLUS

CN Titanium, tetrakis(η^5 -2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)

IT 259881-41-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (prepn. and carbonylation of)

RN 259881-41-9 HCAPLUS

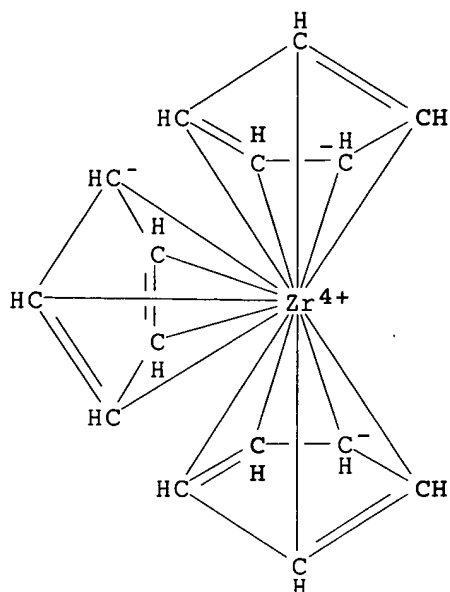
CN Zirconium(1+), tris(η^5 -2,4-cyclopentadien-1-yl)-,
 tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 185549-25-1

CMF C15 H15 Zr

CCI CCS

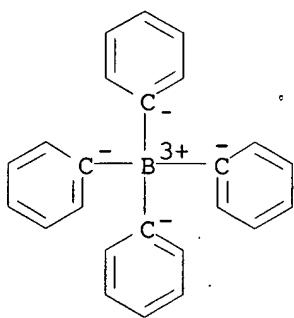


CM 2

CRN 4358-26-3

CMF C24 H20 B

CCI CCS



IT 259881-42-0P 259881-44-2P 259881-46-4P
259881-47-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 259881-42-0 HCAPLUS

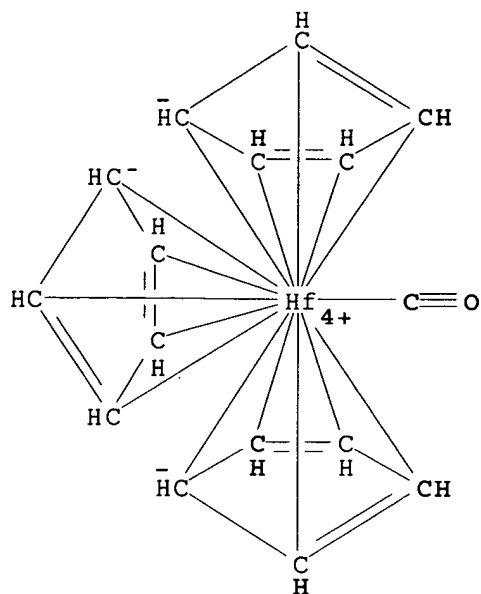
CN Hafnium(1+), carbonyltris(η^5 -2,4-cyclopentadien-1-yl)-,
tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 215596-99-9

CMF C16 H15 Hf O

CCI CCS

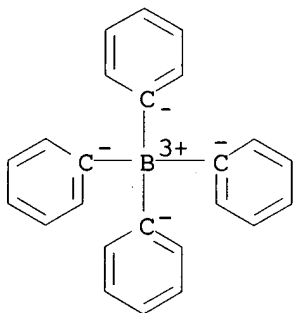


CM 2

CRN 4358-26-3

CMF C24 H20 B

CCI CCS



RN 259881-44-2 HCAPLUS

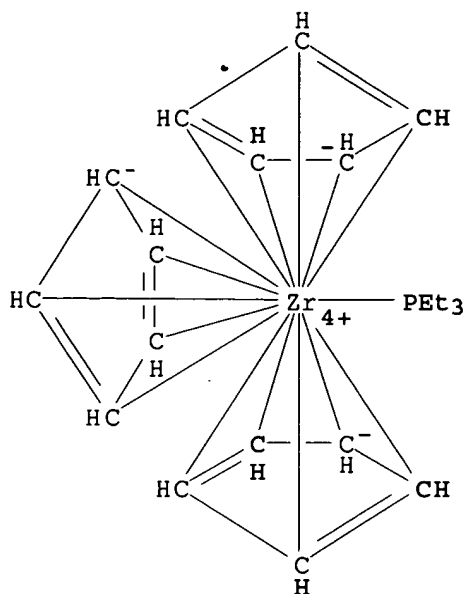
CN Zirconium(1+), tris(η⁵-2,4-cyclopentadien-1-yl)(triethylphosphine)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 259881-43-1

CMF C21 H30 P Zr

CCI CCS

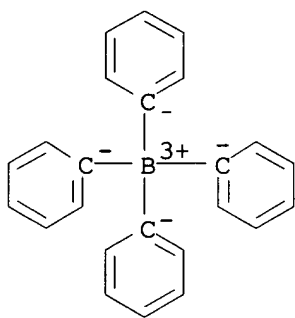


CM 2

CRN 4358-26-3

CMF C24 H20 B

CCI CCS



RN 259881-46-4 HCAPLUS

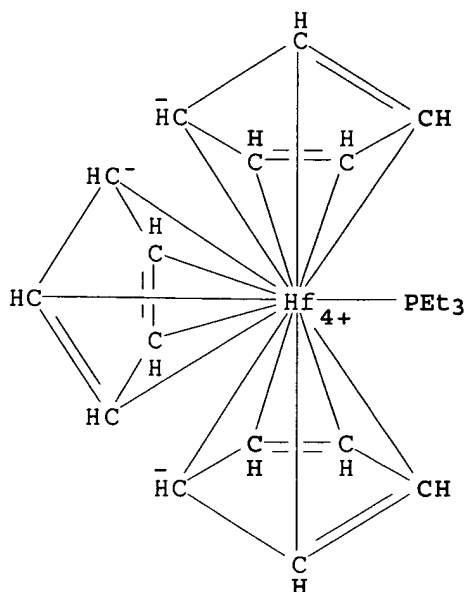
CN Hafnium, tris(η⁵-2,4-cyclopentadien-1-yl) (triethylphosphine)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 259881-45-3

CMF C21 H30 Hf P

CCI CCS

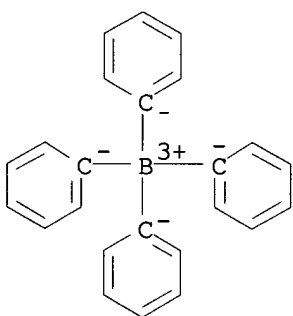


CM 2

CRN 4358-26-3

CMF C24 H20 B

CCI CCS



RN 259881-47-5 HCAPLUS

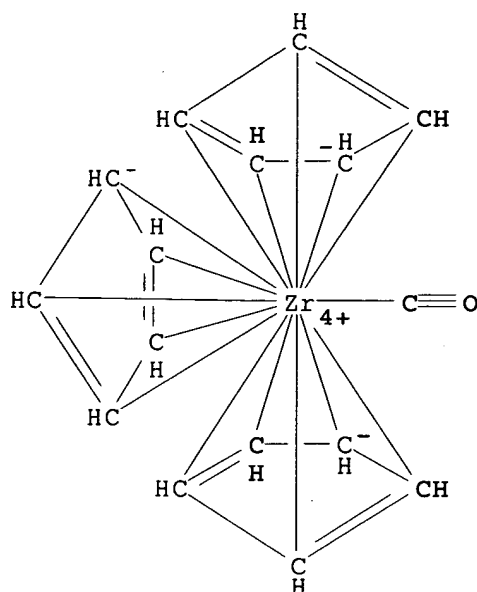
CN Zirconium(1+), carbonyltris(η5-2,4-cyclopentadien-1-yl)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 185549-35-3

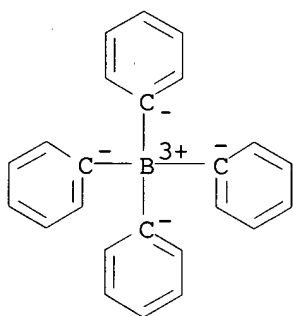
CMF C16 H15 O Zr

CCI CCS

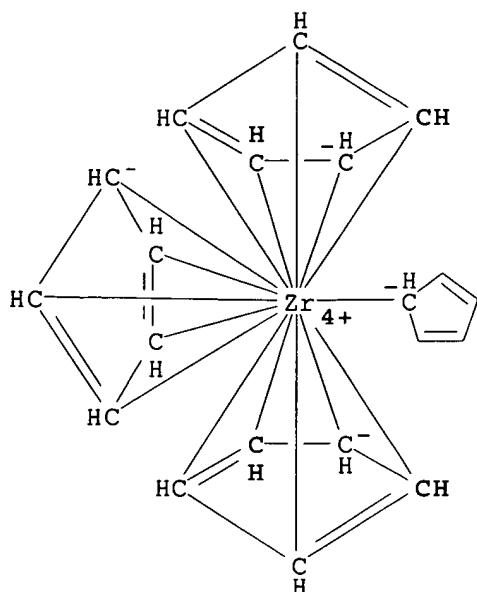


CM 2

CRN 4358-26-3
 CMF C24 H20 B
 CCI CCS



IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (protonation with tributylammonium tetraphenylborate)
 RN 1273-01-4 HCAPLUS
 CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 11079-32-6, Tetrakis(cyclopentadienyl)titanium

RL: RCT (Reactant); RACT (Reactant or reagent)
(double protonation of)

IT 259881-41-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. and carbonylation of)

IT 259881-42-0P 259881-44-2P 259881-46-4P

259881-47-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium 12149-28-9,

Tetrakis(cyclopentadienyl)hafnium

RL: RCT (Reactant); RACT (Reactant or reagent)
(protonation with tributylammonium tetraphenylborate)

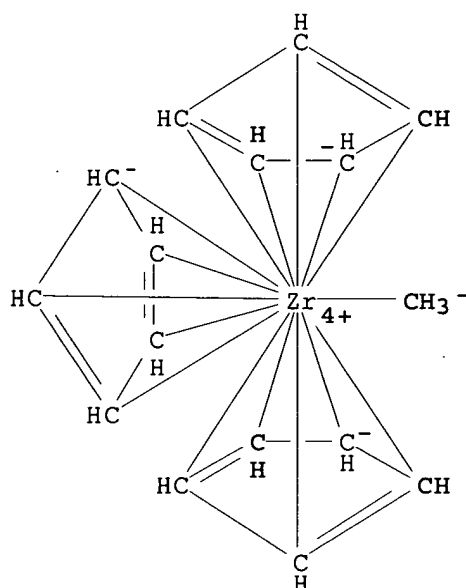
L31 ANSWER 9 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

2000:81709 Document No. 132:222593 (N-pyrrolyl)B(C₆F₅)₂-a new organometallic Lewis acid for the generation of Group 4 metallocene cation complexes. Kehr, Gerald; Frohlich, Roland; Wibbeling, Birgit; Erker, Gerhard (Organisch-Chemisches Institut der Universitat, Munster, D-48149, Germany). Chemistry--A European Journal, 6(2), 258-266 (English) 2000. CODEN: CEUJED. ISSN: 0947-6539. Publisher: Wiley-VCH Verlag GmbH.

AB Treatment of the (C₆F₅)₂BF·OEt₂ (3) complex with N-pyrrolyl Li gives bis(pentafluorophenyl)(N-pyrrolyl)borane (2), a strong organometallic Lewis acid, which was characterized by x-ray diffraction (B-N bond length: 1.401(5) Å). It exhibits a columnar superstructure in the crystal and contains π-stacks of pyrrolyl units. Compd. 2 readily abstrs. alkyl anions from a variety of alkyl Group 4 metallocene-type complexes and leads to the clean formation of the resp. metallocene ions or ion pairs. For example, the treatment of Cp₃ZrCH₃ (9) with 2 transfers a Me anion to yield the ion pair [Cp₃Zr]⁺[(C₄H₄N)BMe(C₆F₅)₂]⁻ (12). The x-ray crystal structure anal. of 12 shows a close contact between Zr and

the pyrrolyl- β -C (2.641(2) Å). The borane 2 adds to (butadiene)zirconocene (13) to yield the betaine system $[\text{Cp}_2\text{Zr}] + [(\text{H}_2\text{C}:\text{CHCHCH}_2)\text{B}(\text{NC}_4\text{H}_4)(\text{C}_6\text{F}_5)_2]^-$ (15). Complex 15 contains a distorted η^3 -allyl moiety inside the metallacyclic framework and it features an internal $\text{Zr} \cdots (\text{pyrrolyl})\text{B}^-$ ion pair interaction with a $\text{Zr} \cdots \text{pyrrolyl}-\alpha\text{-C}$ sepn. of 2.723(3) Å (detd. by x-ray diffraction). From the dynamic NMR spectra of 15 the bond strength of the internal ion pair interaction is $\Delta G_{\text{thermod.diss}}$ (223 K) ≈ 15 kcal mol $^{-1}$. Treatment of dimethylzirconocene (16) with 2 yields the metallocene borate salt $[\text{Cp}_2\text{ZrCH}_3] + [(\text{C}_4\text{H}_4\text{N})\text{BMe}(\text{C}_6\text{F}_5)_2]^-$ (17), which is an active catalyst for the polymn. of ethene.

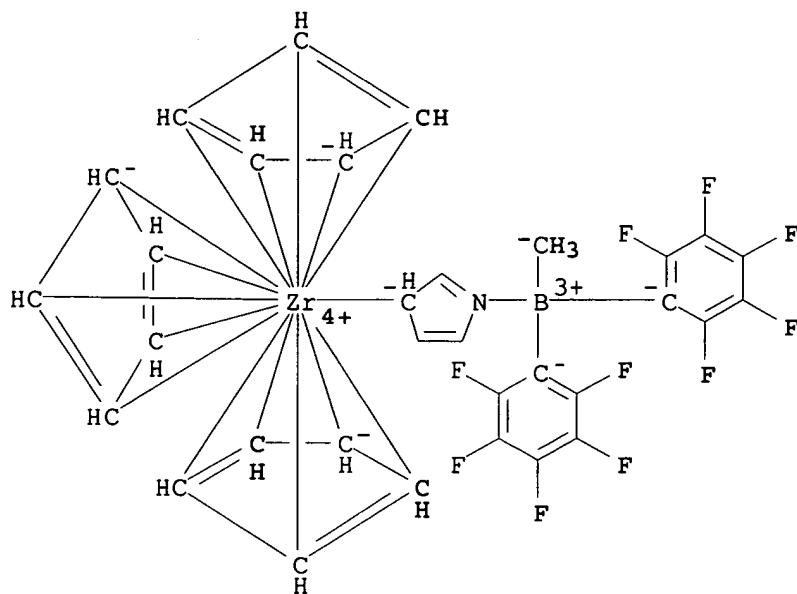
IT 185549-24-0, Tris(η^5 -cyclopentadienyl)(methyl)zirconium
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (carbanion transfer reaction with diaryl(pyrrolyl)borane)
 RN 185549-24-0 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)methyl- (9CI) (CA INDEX NAME)



IT 261347-81-3P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and crystal structure of)
 RN 261347-81-3 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)[methylbis(pentafluorophenyl)boron] [μ -(3H-pyrrol-3-yl- $\kappa\text{C}:\kappa\text{N})$]-, compd. with benzene (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 261347-75-5
 CMF C32 H22 B F10 N Zr
 CCI CCS



CM 2

CRN 71-43-2

CMF C6 H6



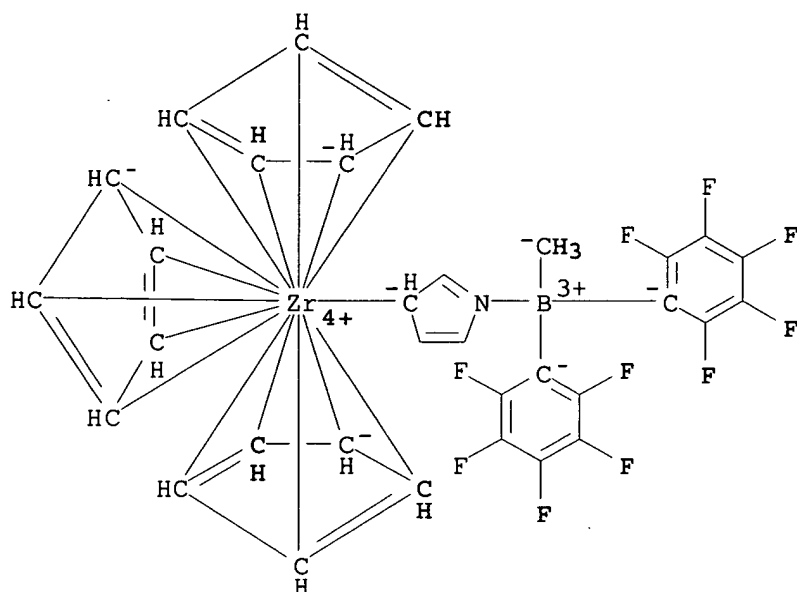
IT 261347-75-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and mol. structure of)

RN 261347-75-5 HCAPLUS

CN Zirconium, tris(eta5-2,4-cyclopentadien-1-yl) [methylbis(pentafluorophenyl)boron] [mu-(3H-pyrrol-3-yl-kappaC:kappaN)]- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 35, 75

IT 12636-72-5, Bis(eta5-cyclopentadienyl)dimethylzirconium

75374-50-4, (eta4-1,3-Butadiene)bis(eta5-cyclopentadienyl)zirconium **185549-24-0**,
Tris(eta5-cyclopentadienyl)(methyl)zirconium

RL: RCT (Reactant); RACT (Reactant or reagent)

(carbanion transfer reaction with diaryl(pyrrolyl)borane)

IT 261347-74-4P, Bis(pentafluorophenyl)(N-pyrrolidinyl)borane

261347-81-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)

(prepn. and crystal structure of)

IT **261347-75-5P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)

(prepn. and mol. structure of)

L31 ANSWER 10 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1999:441553 Document No. 131:199779 Carbon-Fluorine Bond Cleavage by Zirconium Metal Hydride Complexes. Edelbach, Brian L.; Rahman, A. K. Fazlur; Lachicotte, Rene J.; Jones, William D. (Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA). Organometallics, 18(16), 3170-3177 (English) 1999. CODEN: ORGND7. ISSN: 0276-7333. OTHER SOURCES: CASREACT 131:199779. Publisher: American Chemical Society.

AB The Zr hydride dimer [Cp2ZrH2]2 reacts with C6F6 at ambient temp. to give Cp2Zr(C6F5)F as the major product along with Cp2ZrF2, C6F5H and H2. Neither the reaction rate nor the product ratio is affected by changes in H2 pressure or the concn. of C6F6. The reaction follows zero-order kinetics. The new compd. Cp2Zr(C6F5)F was structurally characterized. [Cp2ZrH2]2 reacts with C6F5H to give Cp2Zr(p-C6F4H)F, Cp2ZrF2, C6F4H2, and H2. The Zr hydride Cp3ZrH was structurally characterized and also reacts with C6F6. The products of the reaction are CpH, Cp2Zr(C6F5)F, C6F5H, Cp2ZrF2, Cp4Zr, and Cp3ZrF. The reaction rate is 1st order in [Cp3ZrH] and [C6F6], but

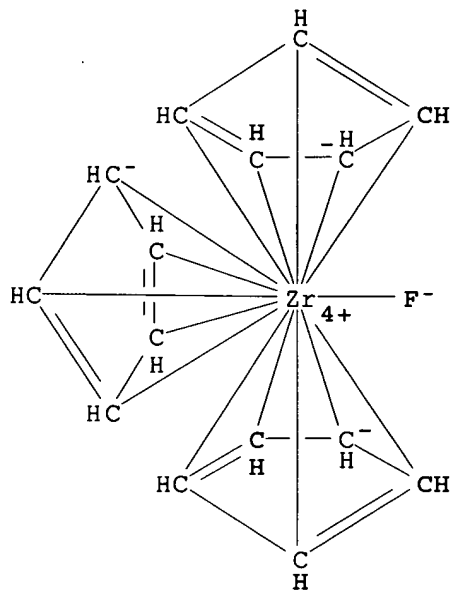
the product ratio is unaffected by the concn. of C₆F₆. Possible mechanisms of these reactions are discussed.

IT 241471-58-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(carbon-fluorine bond cleavage by zirconium metal hydride complexes)

RN 241471-58-9 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)fluoro- (9CI) (CA
INDEX NAME)

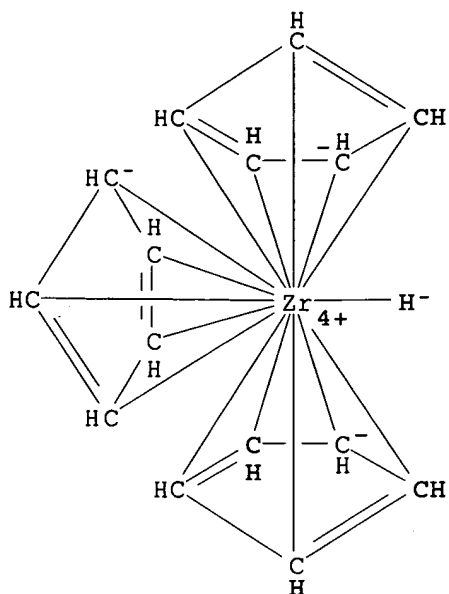


IT 78446-26-1

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(crystal structure; carbon-fluorine bond cleavage by zirconium metal hydride complexes)

RN 78446-26-1 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)hydro- (9CI) (CA
INDEX NAME)

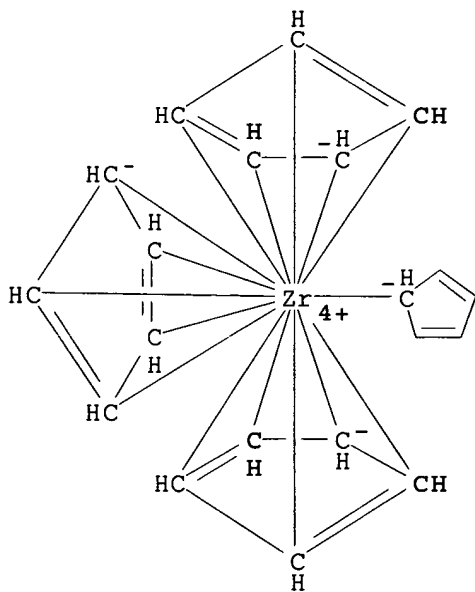


IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with pyridinium poly(hydrogen fluoride))

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η5-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 75

IT 327-54-8P, 1,2,4,5-Tetrafluorobenzene 241471-54-5P 241471-56-7P
241471-58-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(carbon-fluorine bond cleavage by zirconium metal hydride complexes)

IT 78446-26-1

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(crystal structure; carbon-fluorine bond cleavage by zirconium metal hydride complexes)

IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with pyridinium poly(hydrogen fluoride))

L31 ANSWER 11 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1999:290469 Document No. 131:58959 Synthesis of heterobinuclear metallocenes containing bridging ansa-bis- η -cyclopentadienyl ligands. Green, Malcolm L. H.; Popham, Neil H. (Inorganic Chemistry Laboratory, Oxford, OX1 3QR, UK). Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (7), 1049-1060 (English) 1999. CODEN: JCDBT1. ISSN: 0300-9246. Publisher: Royal Society of Chemistry.

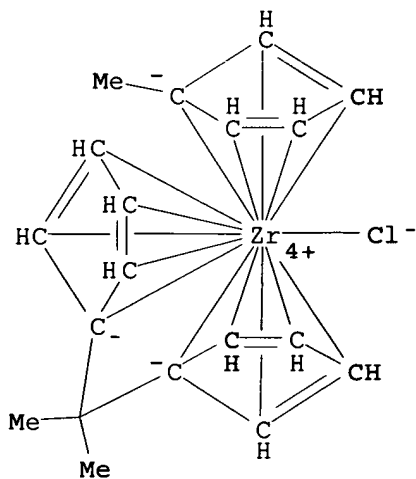
AB Binuclear metallocene derivs. have been prep'd., exemplified by [Cl₂(η -C₅H₅)Zr{ μ -(η -C₅H₄)CMe₂(η -C₉H₆)}Rh(CO)₂], [Cl₂(η -C₅H₅)Zr{ μ -(η -C₅H₄)CMe₂(η -C₉H₆)}Rh(PPh₃)₂], [Cl₂(η -C₅H₅)Zr{ μ -(η -C₅H₄)CMe₂(η -C₉H₆)}Mn(CO)₃], [Cl₂(η -C₅H₅)Zr{ μ -(η -C₅H₄)CMe₂(η -C₉H₆)}Ru(CO)(η -C₄H₇)], [Fe{ μ -(η -C₅H₄)CMe₂(η -C₉H₆)Zr(η -C₅H₅)Cl₂}], [Cl₂(η -C₅H₅)Zr{ μ -(η -C₅H₄)CMe₂(η -C₉H₆)}Co(η -C₅Me₅)], [Cl₂(η -C₅H₅)Zr{ μ -(η -C₅H₄)C(CH₂)₅(η -C₉H₆)}-Zr(η -C₅H₅)Cl₂], [Cl₂(η -C₅H₅)Hf{ μ -(η -C₅H₄)(CH₂)₅C(η -C₉H₆)}Hf(η -C₅H₅)Cl₂]. The tris- η -cyclopentadienyl compds. [Zr{Me₂C(η -C₅H₄)₂(η -C₅H₄Me)Cl}] and the new η -indenyl compd. [Zr{(4-ButC₆H₉)(η -C₅H₄)-(1-CH₆)}(η -C₅H₅)Cl] are also described. The activity of a selection of the binuclear compds. as co-catalysts for ethylene polymn. has been demonstrated.

IT 228088-25-3P

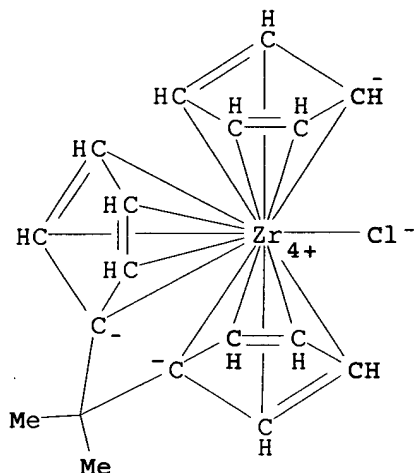
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 228088-25-3 HCAPLUS

CN Zirconium, chloro[(1-methylethylidene)bis(η 5-2,4-cyclopentadien-1-ylidene)][(1,2,3,4,5- η)-1-methyl-2,4-cyclopentadien-1-yl]-(9CI) (CA INDEX NAME)



IT 152337-81-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis of heterobinuclear metallocenes contg. bridging
 ansa-bis-cyclopentadienyl ligands as polymn. catalysts)
 RN 152337-81-0 HCAPLUS
 CN Zirconium, chloro(η^5 -2,4-cyclopentadien-1-yl)[(1-
 methylethylidene)bis(η^5 -2,4-cyclopentadien-1-ylidene)]- (9CI)
 (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 35, 67
 IT 228087-95-4P 228087-97-6P 228087-99-8P 228088-01-5P
 228088-11-7P 228088-20-8P 228088-23-1P **228088-25-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 14100-30-2, Pentacarbonyl(chloro)manganese 14523-22-9,
 Bis(dicarbonyl(chloro)rhodium) 31781-76-7 41066-45-9
 66349-82-4 74353-89-2, Bis(chloro(η^5 -
 pentamethylcyclopentadienyl)cobalt) 129174-25-0 138533-79-6
152337-81-0 154320-40-8 154647-67-3 154647-68-4
 228109-27-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis of heterobinuclear metallocenes contg. bridging
 ansa-bis-cyclopentadienyl ligands as polymn. catalysts)

L31 ANSWER 12 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
 1998:632171 Document No. 129:343556 Comparison of characteristic
 structural features among the triad of tris(cyclopentadienyl) (Group-
 4 metal) complex cations. A combined theoretical and experimental
 study. Jacobsen, Heiko; Berke, Heinz; Brackemeyer, Thomas;
 Eisenblaetter, Tanja; Erker, Gerhard; Froehlich, Roland; Meyer,
 Oliver; Bergander, Klaus (Anorganisch-Chemisches Inst., Univ.
 Zuerich-Irchel, Zurich, CH-8057, Switz.). Helvetica Chimica Acta,
 81(9), 1692-1709 (English) 1998. CODEN: HCACAV. ISSN:
 0018-019X. Publisher: Verlag Helvetica Chimica Acta AG.
 AB A d. functional theory computational chem. study revealed a
 fundamental structural difference between [Ti(Cp)3]⁺ and its
 congeners [Zr(Cp)3]⁺ and [Hf(Cp)3]⁺ (Cp = cyclopentadienyl).
 Whereas the latter 2 contain 3 uniformly η^5 -coordinated Cp

ligands ($3\eta^3$ -structural type), $[\text{Ti}(\text{Cp})_3]^+$ prefers a $2\eta^5\eta^3$ structure. $[\text{Ti}(\text{Cp})_3]^+[\text{B}(\text{C}_6\text{F}_5)_3(\text{Me})]^-$ was exptl. generated by treatment of $[\text{Ti}(\text{Cp})_3(\text{Me})]$ with $\text{B}(\text{C}_6\text{F}_5)_3$. Low-temp. ^1H NMR in CDCl_2 (143 K, 600 MHz) showed a splitting of the Cp resonance into 5 lines in a 2:5:2:5:1 ratio which would be in accord with the theor. predicted $2\eta^5\eta^2$ -type structure of $[\text{Ti}(\text{Cp})_3]^+$. The precursor $[\text{Ti}(\text{Cp})_3(\text{Me})]$ exhibits 2 ^1H NMR Cp resonances in a 10:5 ratio in CD_2Cl_2 at 223 K. Treatment of $[\text{HfCl}(\text{Cp})_2(\text{Me})]$ with NaCp gave $[\text{Hf}(\text{Cp})_3(\text{Me})]$. Its reaction with $\text{B}(\text{C}_6\text{F}_5)_3$ furnished $[\text{Hf}(\text{Cp})_3]^+[\text{B}(\text{C}_6\text{F}_5)_3(\text{Me})]^-$ which reacted with Me_3CNC to give $[\text{Hf}(\text{Cp})_3(\text{C:NCMe}_3)]^+$ {counterion $[\text{B}(\text{C}_6\text{F}_5)_3(\text{Me})]^-$ }, which was characterized by x-ray crystallog. Its $\text{Hf}(\text{Cp}_3)$ moiety is of the $3\eta^5$ -type. The structure is distorted trigonal-pyramidal with an av. D-Hf-D angle of 118.8° and an av. D-Hf-C(1) angle of 96.5° (D denotes the centroids of the Cp rings). It is a typical d⁰-isocyanide complex exhibiting structural parameters of the C:NCMe₃ group {d[C(1)-N(2)] = 1.146 Å; IR: $\sim\nu(\text{C.tplbond.N})$ 2211 cm^{-1} } very similar to free uncomplexed isonitrile. Analogous treatment of $[\text{Hf}(\text{Cp})_3]^+$ with CO yielded the carbonyl (d⁰-Group-4-metal) complex $[\text{Hf}(\text{Cp})_3(\text{CO})]^+[\text{B}(\text{C}_6\text{F}_5)_3(\text{Me})]^-$, which was also characterized by x-ray crystal-structure anal. This complex is also of the $3\eta^5$ -structural type, similar to the previously described cationic complex $[\text{Zr}(\text{Cp})_3(\text{CO})]^+$, and exhibits properties of the CO ligand [d(C-O) = 1.11 Å; IR: $\sim\nu(\text{C-O})$ 2137 cm^{-1}] very similar to the free CO mol.

IT 185549-29-5 185549-35-3 215596-99-9

215597-36-7 215597-41-4 215597-46-9

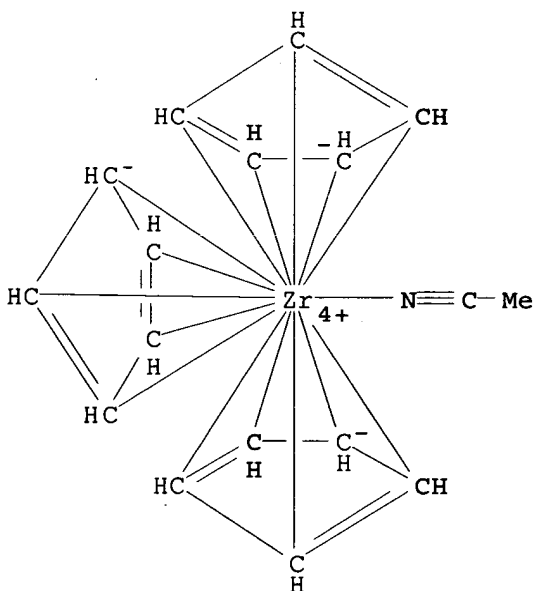
215597-54-9 215597-70-9 215597-76-5

RL: PRP (Properties)

(DFT computational and exptl. comparison of mol. structure and coordinate bond energy)

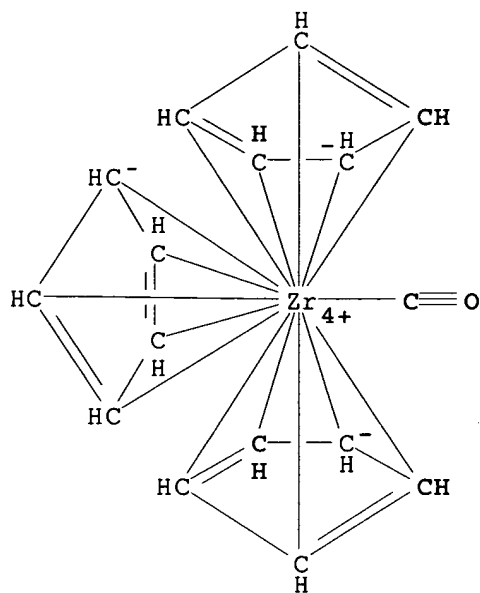
RN 185549-29-5 HCAPLUS

CN Zirconium(1+), (acetonitrile)tris(η^5 -2,4-cyclopentadien-1-yl)-
(9CI) (CA INDEX NAME)

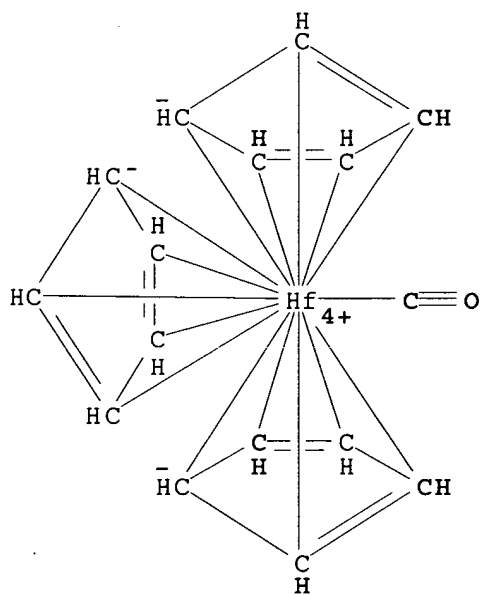


RN 185549-35-3 HCAPLUS

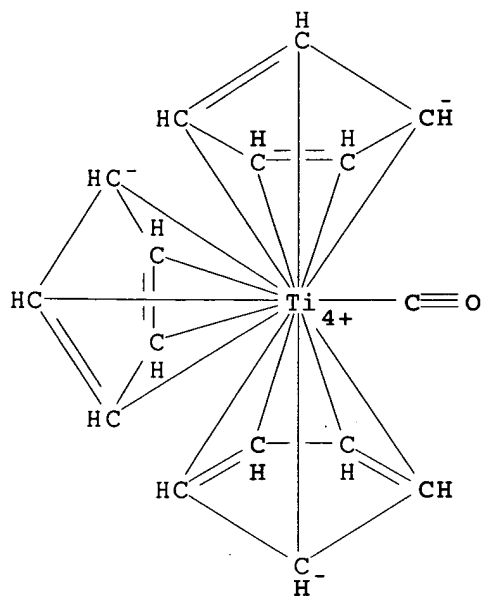
CN Zirconium(1+), carbonyltris(η^5 -2,4-cyclopentadien-1-yl) - (9CI)
(CA INDEX NAME)



RN 215596-99-9 HCAPLUS
CN Hafnium(1+), carbonyltris(η^5 -2,4-cyclopentadien-1-yl) - (9CI)
(CA INDEX NAME)

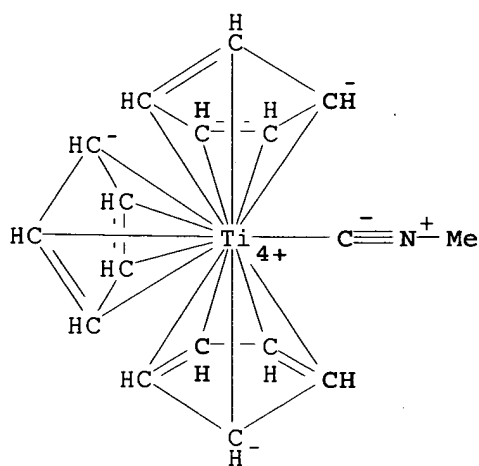


RN 215597-36-7 HCAPLUS
CN Titanium(1+), carbonyltris(η^5 -2,4-cyclopentadien-1-yl) - (9CI)
(CA INDEX NAME)



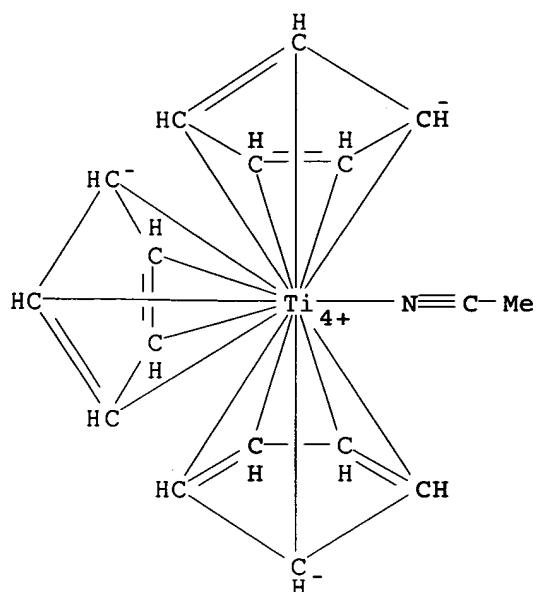
RN 215597-41-4 HCAPLUS

CN Titanium(1+), tris(η5-2,4-cyclopentadien-1-yl)[(isocyano-κC)methane] - (9CI) (CA INDEX NAME)



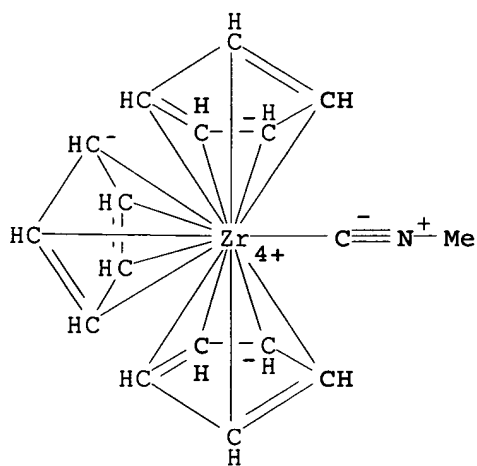
RN 215597-46-9 HCAPLUS

CN Titanium(1+), (acetonitrile)tris(η5-2,4-cyclopentadien-1-yl) - (9CI) (CA INDEX NAME)



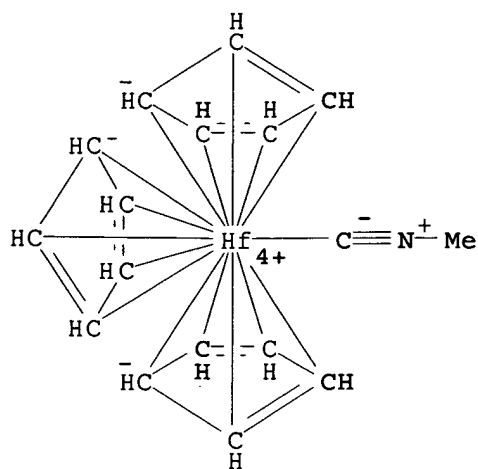
RN 215597-54-9 HCAPLUS

CN Zirconium(1+), tris(η⁵-2,4-cyclopentadien-1-yl) [(isocyano-κC)methane] - (9CI) (CA INDEX NAME)



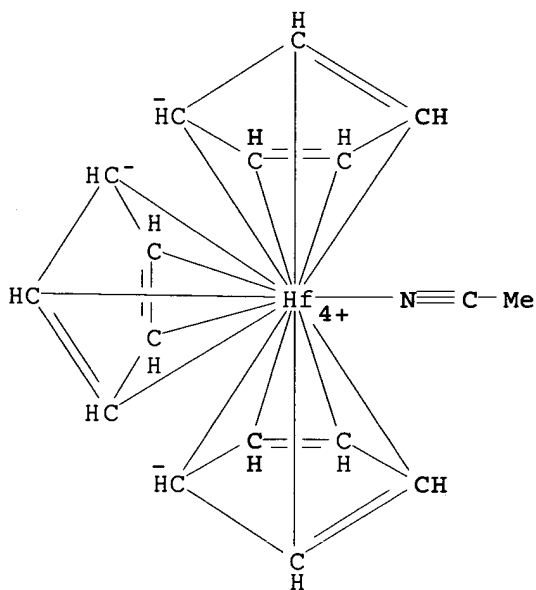
RN 215597-70-9 HCAPLUS

CN Hafnium(1+), tris(η⁵-2,4-cyclopentadien-1-yl) [(isocyano-κC)methane] - (9CI) (CA INDEX NAME)



RN 215597-76-5 HCAPLUS

CN Hafnium(1+), (acetonitrile)tris(η5-2,4-cyclopentadien-1-yl) - (9CI) (CA INDEX NAME)



IT 131323-29-0 185549-25-1 215596-83-1

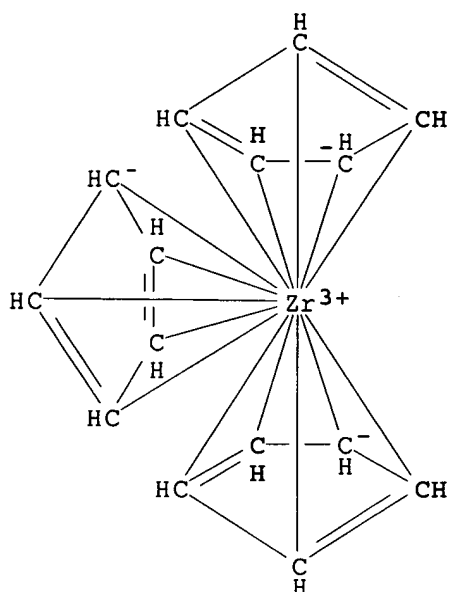
215597-18-5 215597-28-7

RL: PRP (Properties)

(DFT-calcd. and exptl. mol. structure of
tris(cyclopentadienyl)(Group 4 metal) cationic complexes)

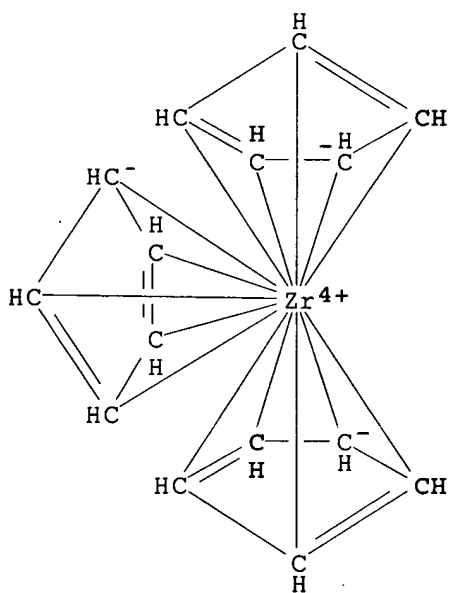
RN 131323-29-0 HCAPLUS

CN Zirconium, tris(η5-2,4-cyclopentadien-1-yl) - (9CI) (CA INDEX NAME)



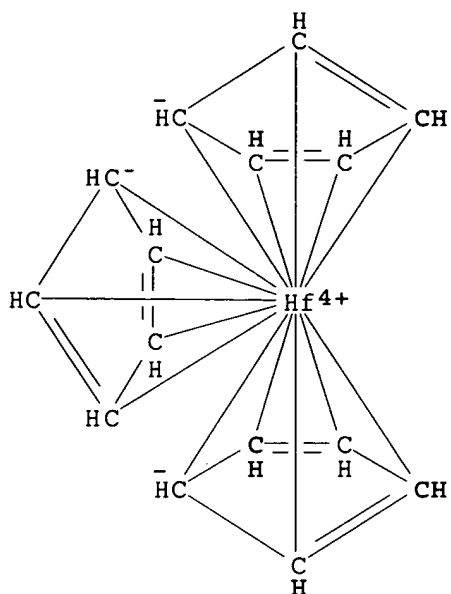
RN 185549-25-1 HCAPLUS

CN Zirconium(1+), tris(η^5 -2,4-cyclopentadien-1-yl) - (9CI) (CA INDEX NAME)

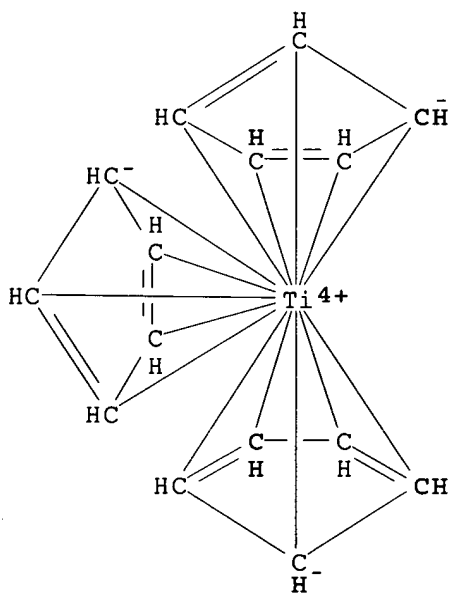


RN 215596-83-1 HCAPLUS

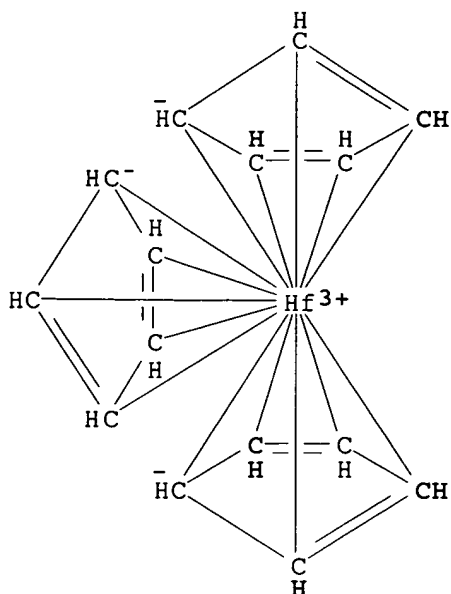
CN Hafnium(1+), tris(η^5 -2,4-cyclopentadien-1-yl) - (9CI) (CA INDEX NAME)



RN 215597-18-5 HCAPLUS
 CN Titanium(1+), tris(η5-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



RN 215597-28-7 HCAPLUS
 CN Hafnium, tris(η5-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



IT 215596-92-2P 215597-00-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(crystal structure; prepn. of tris(cyclopentadienyl)hafnium and -titanium cationic complexes)

RN 215596-92-2 HCAPLUS

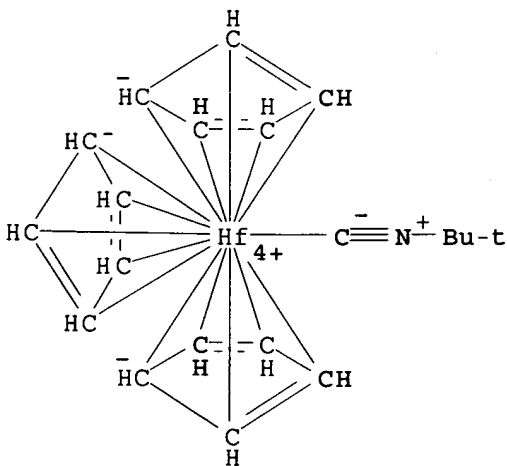
CN Hafnium(1+), tris(η^5 -2,4-cyclopentadien-1-yl) [2-(isocyano- κ C)-2-methylpropane]-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 215596-91-1

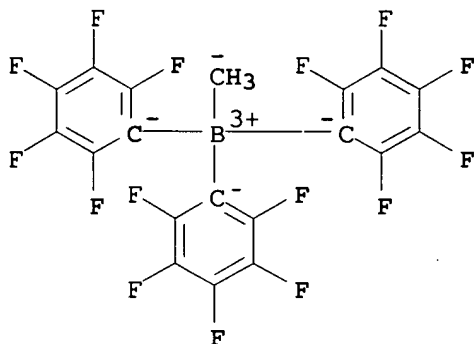
CMF C20 H24 Hf N

CCI CCS



CM 2

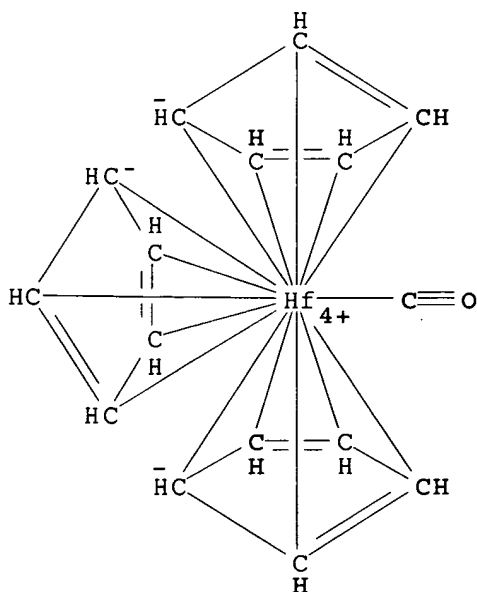
CRN 133445-48-4
 CMF C19 H3 B F15
 CCI CCS



RN 215597-00-5 HCAPLUS
 CN Hafnium(1+), carbonyltris(η^5 -2,4-cyclopentadien-1-yl)-,
 (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

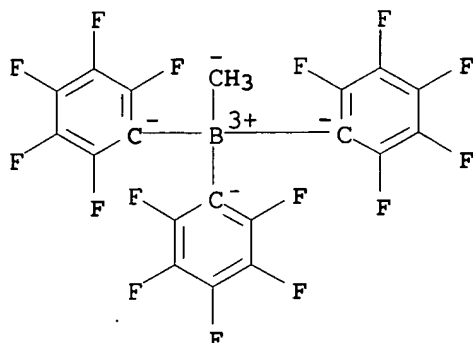
CRN 215596-99-9
 CMF C16 H15 Hf O
 CCI CCS



CM 2

CRN 133445-48-4

CMF C19 H3 B F15
CCI CCS

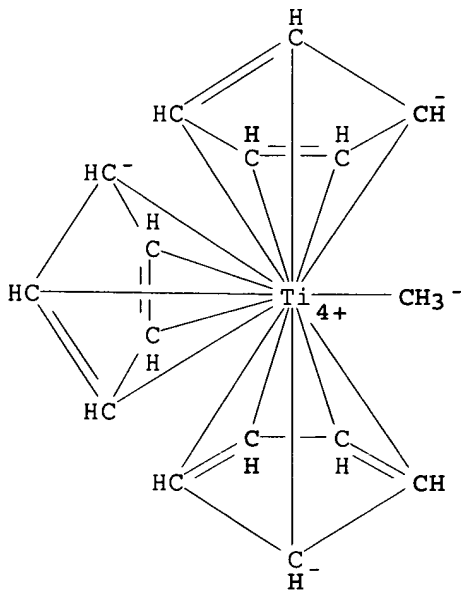


IT 215596-72-8P 215596-78-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(prepn. of tris(cyclopentadienyl)hafnium and -titanium cationic
complexes)

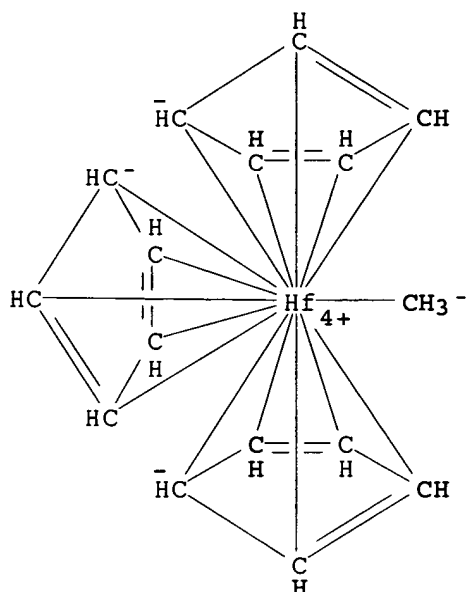
RN 215596-72-8 HCAPLUS

CN Titanium, tris(η^5 -2,4-cyclopentadien-1-yl)methyl- (9CI) (CA
INDEX NAME)



RN 215596-78-4 HCAPLUS

CN Hafnium, tris(η^5 -2,4-cyclopentadien-1-yl)methyl- (9CI) (CA
INDEX NAME)



IT 215596-84-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of tris(cyclopentadienyl)hafnium and -titanium cationic
complexes)

RN 215596-84-2 HCAPLUS

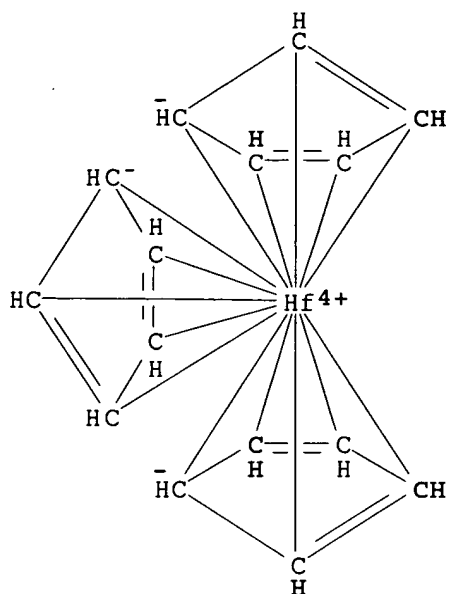
CN Hafnium(1+), tris(η^5 -2,4-cyclopentadien-1-yl)-,
(T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 215596-83-1

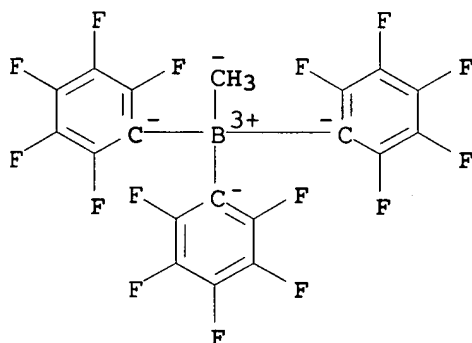
CMF C15 H15 Hf

CCI CCS



CM 2

CRN 133445-48-4
 CMF C19 H3 B F15
 CCI CCS



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 75

IT 185549-29-5 185549-35-3 215596-99-9

215597-36-7 215597-41-4 215597-46-9

215597-54-9 215597-70-9 215597-76-5

RL: PRP (Properties)

(DFT computational and exptl. comparison of mol. structure and coordinate bond energy)

IT 52700-41-1 52700-41-1 131323-29-0 185549-25-1

215596-83-1 215597-07-2 215597-18-5

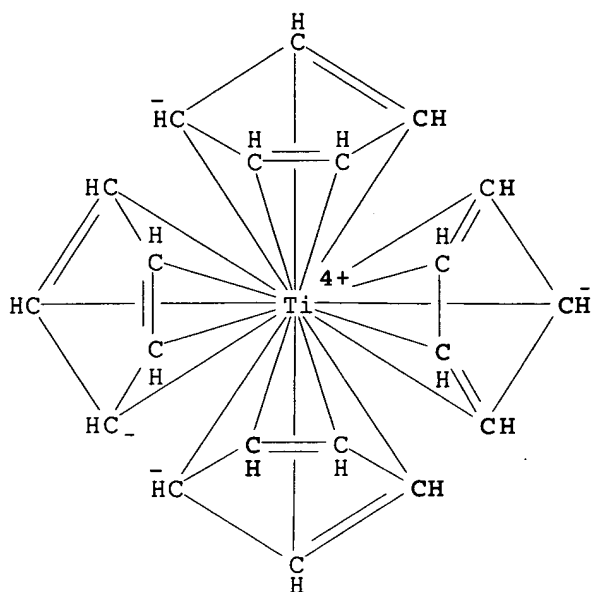
215597-28-7 215597-86-7 215597-91-4 215597-95-8

215598-00-8

RL: PRP (Properties)

(DFT-calcd. and exptl. mol. structure of

- tris(cyclopentadienyl)(Group 4 metal) cationic complexes)
- IT 215596-92-2P 215597-00-5P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (crystal structure; prepn. of tris(cyclopentadienyl)hafnium and -titanium cationic complexes)
- IT 215596-72-8P 215596-78-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of tris(cyclopentadienyl)hafnium and -titanium cationic complexes)
- IT 215596-84-2P 215597-08-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of tris(cyclopentadienyl)hafnium and -titanium cationic complexes)
- L31 ANSWER 13 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
 1998:227746 Document No. 128:308513 Organometallics of transition metals in supercritical carbon dioxide. Solubilities, reactions, catalysis. Kreher, Ulf; Schebesta, Sebastian; Walther, Dirk (Institut Anorganische Analytische Chemie, Friedrich-Schiller-Universitaet, Jena, D-07743, Germany). Zeitschrift fuer Anorganische und Allgemeine Chemie, 624(4), 602-612 (German) 1998. CODEN: ZAACAB. ISSN: 0044-2313. Publisher: Johann Ambrosius Barth.
- AB Monomeric compds. of the type Cp₂M (M = Fe, Co, Ni etc.) are sol. in liq. or supercrit. CO₂ without any reaction with the solvent. The polymeric compds. zirconocene and manganocene form insol. CO₂ insertion products with CO₂. Homoleptic metal carbonyls as well as a no. of ligand-stabilized metal carbonyls are also sol. in scCO₂. Fe(CO)₅ reacts photochem. in this solvent to Fe₂(CO)₉ and thermally to Fe₃(CO)₁₂. The highly reactive (cdt)Ni(0) (cdt = 1,5,9-cyclododecatriene) is sol. in liq. CO₂. A reaction with the solvent was not obsd. In scCO₂ soln., (cdt)Ni reacts thermally to form Ni after a short time. CpCo(cod) catalyzes slowly the cyclo-cooligomerization of 3-hexyne with MeCN to form 2,3,4,5-tetraethyl-6-methylpyridine. HC.tplbond.CHCH₂OH reacts under formation of cyclotetramers with a selectivity of 90% using (cod)₂Ni or (cdt)Ni as catalysts. 3-Hexyne reacts in and with CO₂ under selective formation of tetraethyl-2-pyrone when the catalyst system R₃P/(cod)₂Ni (R = Me, Et) is used. In-situ IR shows that the catalytically active species will be deactivated by formation of Ni carbonyl complexes. The catalytic oxidn. of cyclooctene to cyclooctene oxide with Me₃COOH using Ti(OCHMe₂)₄ as sol. catalyst proceeds less selectively. However, in the presence of Mo(CO)₆ the epoxide is formed in good yields and with high selectivity.
- IT 11079-32-6, Tetracyclopentadienyltitanium
 RL: PRP (Properties)
 (soly. and stability in liq. and supercrit. carbon dioxide and in Freon)
- RN 11079-32-6 HCAPLUS
 CN Titanium, tetrakis(η⁵-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



CC 29-1 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 67, 68, 78

IT 102-54-5, Ferrocene 136-52-7 1271-19-8, Titanocene dichloride
 1271-28-9, Nickelocene 1271-55-2, Acetylferrocene 1271-66-5,
 Dimethyltitanocene 1273-09-2, Diphenyltitanocene 1277-43-6,
 Cobaltocene 1277-47-0, Vanadocene 3264-82-2,
 Bis(acetylacetonate)nickel 11079-32-6,
 Tetracyclopentadienyltitanium 11136-36-0, Decamethyltitanocene
 dichloride 12079-65-1, Tricarbonylcyclopentadienylmanganese
 12079-73-1, Tricarbonylcyclopentadienylrhodium 12082-08-5,
 Tricarbonylbenzenechromium 12112-97-9 12116-83-5, Zirconocene
 12126-50-0, Decamethylferrocene 12130-66-4, Bis(1,5-
 cyclooctadiene)platinum 12130-88-0, Tricarbonyl(pentamethylcyclope
 ntadienyl)rhodium 12152-72-6, Cyclohexadienetricarbonyl iron
 13463-40-6, Pentacarbonyliron 14285-68-8, Decacarbonyldirhenium
 14694-95-2, Tris(triphenylphosphine)rhodium chloride 15133-82-1,
 Tetrakis(triphenylphosphine)nickel 15243-33-1,
 Dodecacarbonyltriruthenium 15321-51-4, Nonacarbonyldiiron
 17685-52-8, Dodecacarbonyltriiron 36100-16-0 51320-65-1,
 Tetrakis(triethylphosphine)nickel 60324-03-0, Dimesitylmolybdenum
 dioxide 61930-21-0 73138-26-8, Manganocene 79004-93-6
 101077-61-6, (1,5-Cyclooctadiene)bis(trimethylphosphine)nickel
 122093-43-0, Cyclopentadienylrhodium trioxide 206272-33-5

RL: PRP (Properties)

(soly. and stability in liq. and supercrit. carbon dioxide and in
 Freon)

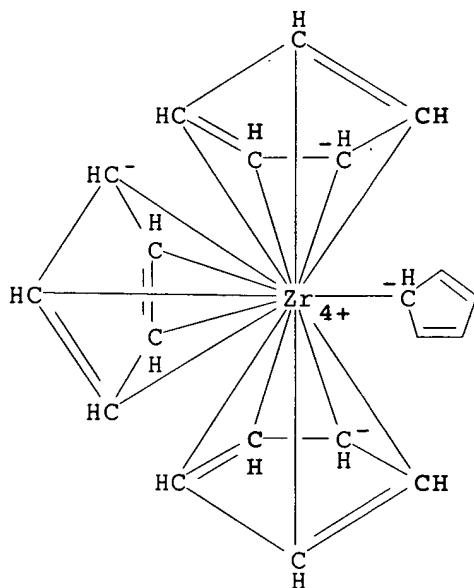
L31 ANSWER 14 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1998:200207 Document No. 128:282915 The tetracyclopentadienyls of
 titanium, zirconium and hafnium: new synthetic procedures and
 reactivity. Calderazzo, Fausto; Englert, Ulli; Pampaloni, Guido;
 Tripepi, Giovanna (Dipartimento di Chimica e Chimica Industriale,
 Universita de Pisa, Pisa, I-56126, Italy). Journal of
 Organometallic Chemistry, 555(1), 49-56 (English) 1998.
 CODEN: JORCAI. ISSN: 0022-328X. Publisher: Elsevier Science S.A..

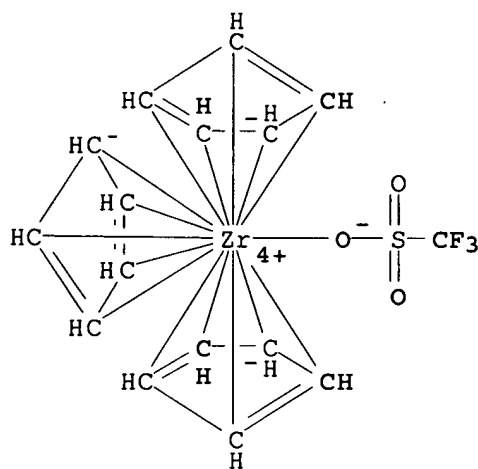
AB In toluene as medium, the tetra(cyclopentadienyl) derivs. of Group 4

elements, MCp_4 ($M = \text{Ti, Zr, Hf}$), were prep'd. in high yields from MCp_2Cl_2 and NaCp . The reactivity of ZrCp_4 with species contg. active protons such as Ph_3SiOH or strong acids was studied. Substituted bis(cyclopentadienyl) derivs. were produced except in the case of the reaction between ZrCp_4 and $\text{CF}_3\text{SO}_3\text{H}$. In this case, the tris(cyclopentadienyl) deriv. $\text{ZrCp}_3(\text{CF}_3\text{SO}_3)$ was obtained as a pale yellow cryst. material, reactive with H_2O to give the μ -oxo deriv. of Zr(IV) , $[\text{ZrCp}_2(\text{CF}_3\text{SO}_3)]_2\text{O}$, which was characterized by std. methods and by x-ray diffraction. Crystal data: $\text{C}_{22}\text{H}_{20}\text{F}_6\text{O}_7\text{S}_2\text{Zr}_2$, $M = 756.96 \text{ g mol}^{-1}$, monoclinic, space group $\text{C}2/c$, $a 19.525(4)$, $b 9.028(2)$, $c 16.152(5) \text{ \AA}$, $\beta 107.31(2)^\circ$, $Z = 4$, $d_c = 1.850 \text{ g cm}^{-3}$, $\lambda(\text{Cu-K}\alpha) = 1.54184 \text{ \AA}$, $T = 291 \text{ K}$, $\mu = 85.66 \text{ cm}^{-1}$, $F(000) = 1496$, $R = 0.054$, $R_w = 0.049$.

- IT **1273-01-4P**, (η^1 -Cyclopentadienyl)tris(η^5 -cyclopentadienyl)zirconium
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and reactions of)
 RN 1273-01-4 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



- IT **205746-14-1P**, Tris(η^5 -cyclopentadienyl)(trifluoromethanesulfonato)zirconium
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. from tetracyclopentadienyl, reaction with triflic acid and hydrolysis of)
 RN 205746-14-1 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)(trifluoromethanesulfonato- κO)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

IT 1273-01-4P, (η^1 -Cyclopentadienyl)tris(η^5 -cyclopentadienyl)zirconium

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and reactions of)

IT 205746-14-1P, Tris(η^5 -cyclopentadienyl)(trifluoromethane sulfonato)zirconium

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. from tetracyclopentadienyl, reaction with triflic acid and hydrolysis of)

L31 ANSWER 15 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1998:200162 Document No. 128:270687 Cyclopentadienyl-diethylcarbamato derivatives of zirconium(IV) and hafnium(IV), $[M(C_5H_5)(O_2CNEt_2)_3]$: synthesis and use as precursors for chemical implantation on a silica surface. Abis, Luigi; Calderazzo, Fausto; Maichle-Mossmer, Cacilia; Pampaloni, Guido; Strahle, Joachim; Tripepi, Giovanna (Istituto Guido Donegani-Enichem, Novara, I-28100, Italy). Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (5), 841-845 (English) 1998. CODEN: JCDTBI. ISSN: 0300-9246. Publisher: Royal Society of Chemistry.

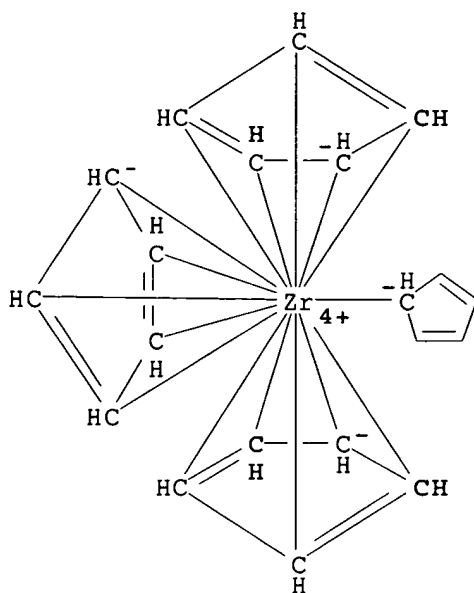
AB Reaction of $Mg(C_5H_5)_2$ with the homoleptic diethylcarbamato derivs. of zirconium(IV) or hafnium(IV), $M(O_2CNEt_2)_4$, gave the mixed cyclopentadienyl-diethylcarbamato complexes $[M(C_5H_5)(O_2CNEt_2)_3]$. These derivs. have also been obtained by reaction of $Fe(O_2CNEt_2)_2$ with $M(C_5H_5)_4$ in the appropriate stoichiometric ratio. The compd. $[Zr(C_5H_5)(O_2CNEt_2)_3]$ crystallizes in the space group P_{4121} , $Z = 2$, $a = 9.734(4)$, $b = 10.234(2)$, $c = 12.948(6)$ Å; $\alpha = 83.41(4)$, $\beta = 86.13(4)$ and $\gamma = 67.43(3)^\circ$. On reaction of $[Zr(C_5H_5)(O_2CNEt_2)_3]$ with dehydrated silica, 1 mol of CO_2 per zirconium was evolved. The organometallic fragment $Zr(C_5H_5)(O_2CNEt_2)_2$ grafted on silica has been characterized by anal. methods and by CP MAS ^{13}C NMR spectroscopy.

IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with iron diethylcarbamato complex)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium 12149-28-9,
Tetrakis(cyclopentadienyl)hafnium

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with iron diethylcarbamato complex)

L31 ANSWER 16 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1998:194856 Document No. 128:295075 Homo- and hetero-binuclear
ansa-metallocenes of the group 4 transition metals as homogeneous
co-catalysts for the polymerization of ethene and propene. Yan,
Xuefeng; Chernega, Alexander; Green, Malcolm L. H.; Sanders, John;
Souter, Joanne; Ushioda, Tsutomu (Inorganic Chemistry Laboratory,
Oxford, OX1 3QR, UK). Journal of Molecular Catalysis A: Chemical,
128(1-3), 119-141 (English) 1998. CODEN: JMCCF2. ISSN:
1381-1169. Publisher: Elsevier Science B.V..

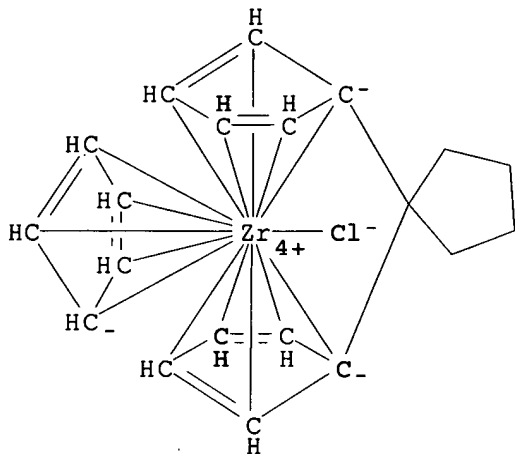
AB The compds. $[M\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}(\eta\text{-C}_5\text{H}_5)\text{Cl}]$ ($M = \text{Zr}, \text{Hf}$),
 $[M\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}(\eta\text{-C}_5\text{H}_5)\text{Me}]$, $[(\eta\text{-C}_5\text{H}_5)\text{MCl}_2\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}\text{MCl}_2(\eta\text{-C}_5\text{H}_5)]$,
 $[(\eta\text{-C}_5\text{H}_5)\text{ZrCl}_2\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}\text{ZrCl}_2(\eta\text{-C}_5\text{H}_5)]$, $[(\eta\text{-C}_5\text{H}_5)\text{MMe}_2\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}\text{MMe}_2(\eta\text{-C}_5\text{H}_5)]$,
 $[(\eta\text{-C}_5\text{H}_5)\text{ZrCl}_2\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}\text{HfCl}_2(\eta\text{-C}_5\text{H}_5)]$,
 $[(\eta\text{-C}_5\text{H}_5)\text{MCl}_2\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}\text{Rh}(\eta\text{-C}_8\text{H}_{12})]$,
 $[(\eta\text{-C}_5\text{H}_5)\text{ZrCl}_2\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}\text{TiCl}_3]$, $[(\eta\text{-C}_5\text{H}_5)\text{ZrMe}_2\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}\text{HfMe}_2(\eta\text{-C}_5\text{H}_5)]$,
 $[(\eta\text{-C}_5\text{H}_5)\text{MMe}_2\{(\text{CH}_2)_4\text{C}(\eta\text{-C}_5\text{H}_4)_2\}\text{Rh}(\eta\text{-C}_8\text{H}_{12})]$ were prepd.
and characterized. The crystal structure was detd. for some of the
Zr complexes. The catalytic activity of several
ansa-metallocenes/MAO was evaluated in polymn. of ethene and
propene. All the catalyst system remained active, however the
activity was lower in propene polymn. than for ethene polymn. The
systems which lack a high degree of stereospecificity also showed
poor activity, attributed to steric hindrance effects.

IT 206071-36-5P

RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepn. and catalytic activity of binuclear hafnium and rhodium and zirconium ansa-metallocenes in polymn. of ethene and propene)

RN 206071-36-5 HCAPLUS

CN Zirconium, chloro(η^5 -2,4-cyclopentadien-1-yl)[cyclopentylidenebis(η^5 -2,4-cyclopentadien-1-ylidene)]- (9CI)
 (CA INDEX NAME)

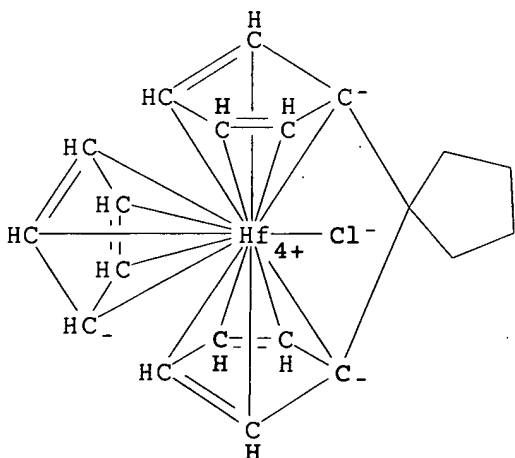


IT 206071-37-6P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepn. and catalytic activity of binuclear hafnium and rhodium and zirconium ansa-metallocenes in polymn. of ethene and propene)

RN 206071-37-6 HCAPLUS

CN Hafnium, chloro(η^5 -2,4-cyclopentadien-1-yl)[cyclopentylidenebis(η^5 -2,4-cyclopentadien-1-ylidene)]- (9CI)
 (CA INDEX NAME)



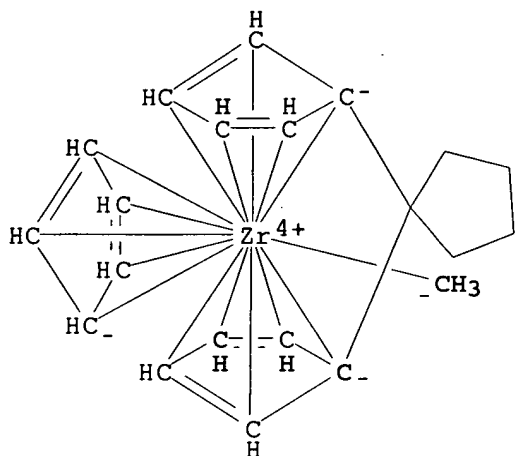
IT 206071-38-7P 206071-39-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)

(prepn. and catalytic activity of binuclear hafnium and rhodium
 and zirconium ansa-metallocenes in polymn. of ethene and propene)

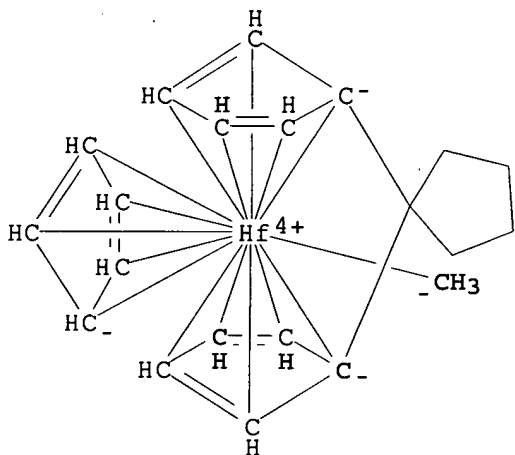
RN 206071-38-7 HCAPLUS

CN Zirconium, (η^5 -2,4-cyclopentadien-1-yl) [cyclopentylidenebis(η^5 -2,4-cyclopentadien-1-ylidene)]methyl-
 (9CI) (CA INDEX NAME)



RN 206071-39-8 HCAPLUS

CN Hafnium, (η^5 -2,4-cyclopentadien-1-yl) [cyclopentylidenebis(η^5 -
 2,4-cyclopentadien-1-ylidene)]methyl- (9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 29, 67

IT 206071-36-5P 206071-50-3P

RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN
 (Synthetic preparation); PREP (Preparation); RACT (Reactant or
 reagent); USES (Uses)

(prepn. and catalytic activity of binuclear hafnium and rhodium
 and zirconium ansa-metallocenes in polymn. of ethene and propene)

IT 206071-37-6P 206071-40-1P 206071-41-2P 206071-46-7P

206071-52-5P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. and catalytic activity of binuclear hafnium and rhodium and zirconium ansa-metallocenes in polymn. of ethene and propene)

IT 141525-86-2P 162609-30-5P 206071-31-0P 206071-34-3P

206071-38-7P 206071-39-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and catalytic activity of binuclear hafnium and rhodium and zirconium ansa-metallocenes in polymn. of ethene and propene)

L31 ANSWER 17 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1997:679907 Document No. 127:278264 The Titanocene Dicarbonyl Dication [TiCp2(CO)2]2+. Calderazzo, Fausto; Pampaloni, Guido; Tripepi, Giovanna (Dipartimento di Chimica e Chimica Industriale, Universita di Pisa, Pisa, I-56126, Italy). Organometallics, 16(23), 4943-4944 (English) 1997. CODEN: ORGND7. ISSN: 0276-7333. OTHER

SOURCES: CASREACT 127:278264. Publisher: American Chemical Society.

AB Two-electron oxidn. of TiCp2(CO)2 with FeCp2[BPh4] or double protonation of TiCp4 with [Bu3NH][BPh4] in toluene affords an exceedingly moisture-sensitive solid which was isolated and identified as the tetraphenylborato deriv. of the titanocene dicarbonyl dication [TiCp2(CO)2][BPh4]2 from both spectroscopic data and reactivity.

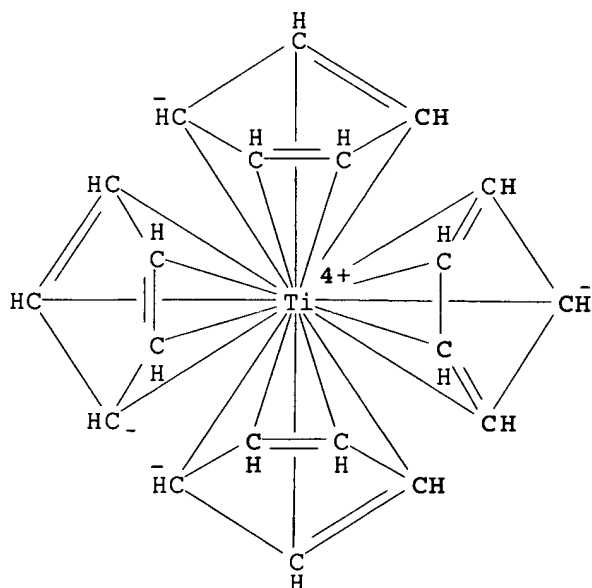
IT 11079-32-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. and reactions of titanocene dicarbonyl dication)

RN 11079-32-6 HCAPLUS

CN Titanium, tetrakis(η5-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 1277-43-6, Cobaltocene 11057-46-8, Ferrocenium tetraphenylborate

11079-32-6 21050-13-5 64167-39-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. and reactions of titanocene dicarbonyl dication)

L31 ANSWER 18 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1997:666419 Document No. 127:307450 Sterically overloaded indenyl complexes of zirconium and hafnium. Schmid, Claudia; Alt, Helmut G.; Milius, Wolfgang (Laboratorium fuer Anorganische Chemie der Universitaet Bayreuth, Postfach 10 21 51, Bayreuth, D-95440, Germany). Journal of Organometallic Chemistry, 544(1), 139-142 (German) 1997. CODEN: JORCAI. ISSN: 0022-328X. Publisher: Elsevier.

AB The reaction of zirconocene dichloride, Cp_2ZrCl_2 , and bis(indenyl) metal dichloride, Ind_2MCl_2 ($\text{M} = \text{Zr}, \text{Hf}$), with one and two equiv., resp., of indenyl or fluorenyl Li leads to sterically crowded complexes with three or four potential π -ligands ($\text{Cp}_2\text{Zr}(\text{Ind})\text{Cl}$, $\text{Cp}_2\text{Zr}(\text{Ind})_2$, Ind_3ZrCl , Ind_3HfCl (4), $\text{Ind}_2\text{Zr}(\text{Flu})\text{Cl}$). Compd. 4 was characterized by an x-ray structure anal.

IT 197503-10-9P, Chlorotris(η^5 -indenyl)hafnium

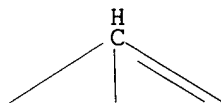
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and crystal structure of)

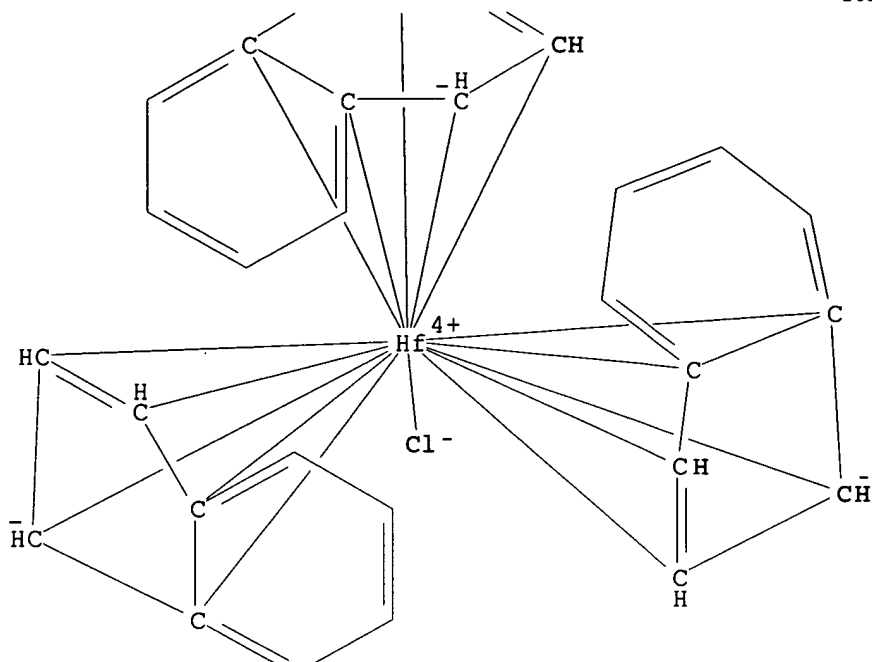
RN 197503-10-9 HCAPLUS

CN Hafnium, chlorotris[(1,2,3,3a,7a- η)-1H-inden-1-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



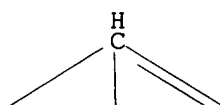
PAGE 2-A



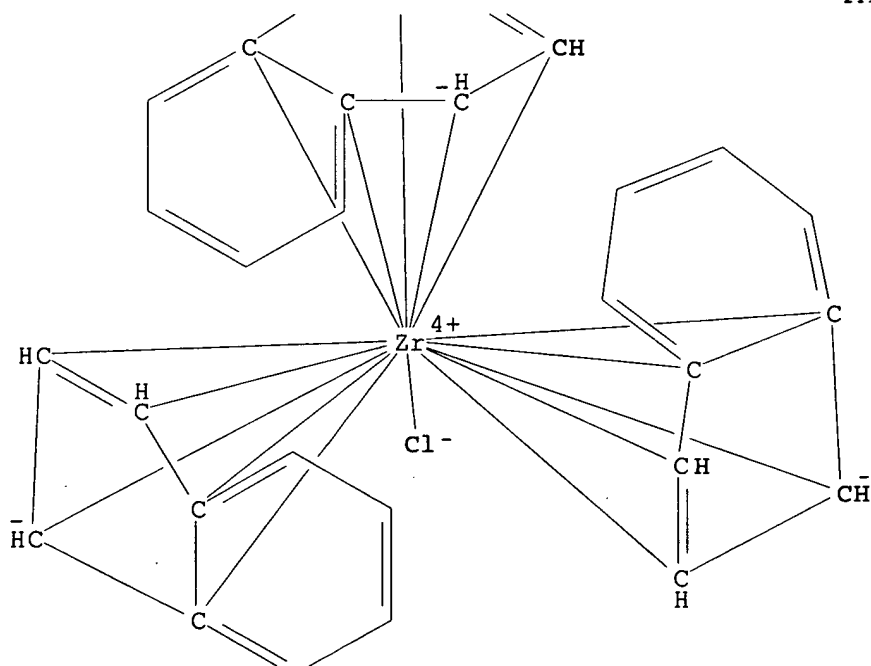
PAGE 3-A

IT 197503-09-6P, Chlorotris(η^5 -indenyl)zirconium
 RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
 (prepn. and hindered rotation in)
 RN 197503-09-6 HCAPLUS
 CN Zirconium, chlorotris[(1,2,3,3a,7a- η)-1H-inden-1-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



PAGE 3-A

CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75

IT 197503-10-9P, Chlorotris(η^5 -indenyl)hafnium
RL: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)
(prepn. and crystal structure of)

IT 197503-09-6P, Chlorotris(η^5 -indenyl)zirconium
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic
preparation); PREP (Preparation); PROC (Process)
(prepn. and hindered rotation in)

L31 ANSWER 19 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
1997:429057 Document No. 127:176521 Cp3Zr(acetonitrile)+. Structure of
an electron-rich organometallic d0-cation. Brackemeyer, Thomas;
Erker, Gerhard; Frohlich, Roland; Prigge, Jorg; Peuchert, Ulrich
(Organisch-Chemisches Inst., Univ. Munster, Muenster, D-48149,
Germany). Chemische Berichte/Recueil, 130(7), 899-902 (English)
1997. CODEN: CHBRFW. Publisher: Wiley-VCH.

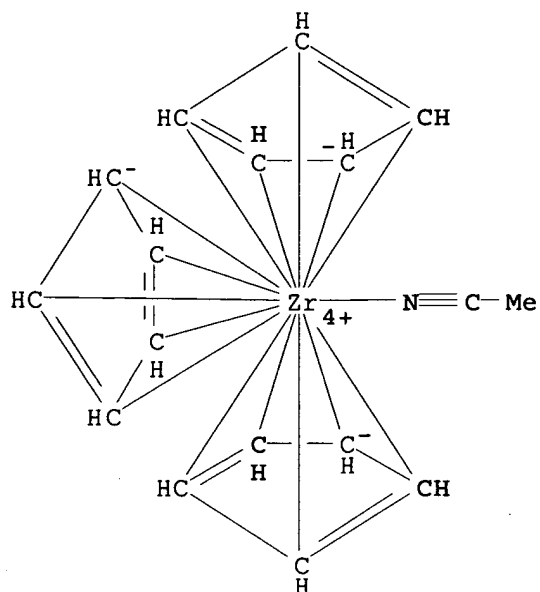
AB [Cp3Zr(NCMe)]+[MeB(C6F5)3]- was prepd. by treatment of Cp3ZrMe with
B(C6F5)3 followed by the addn. of MeCN. X-ray crystal structure
anal. shows 3 uniformly coordinated η^5 -cyclopentadienyl ligands
around the Zr atom. The MeCN ligand is end-on coordinated. In the
linear [Zr]-N.tplbond.C-Me unit the C.tplbond.N triple bond [N-C2
1.126(5) Å] is slightly shorter than the free MeCN mol.
[dC.tplbond.N = 1.141(2) Å], the structure of which was detd. as
a ref. by x-ray diffraction of a crystal obtained by IR
laser-induced zone melting on the diffractometer.

IT 193899-31-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)
(crystal structure; prepn. and structure of
tris(cyclopentadienyl)zirconium acetonitrile complex)

RN 193899-31-9 HCAPLUS
CN Zirconium(1+), (acetonitrile)tris(η^5 -2,4-cyclopentadien-1-yl)-,
(T-4)-methyltris(pentafluorophenyl)borate(1-), compd. with
dichloromethane (1:1) (9CI) (CA INDEX NAME)

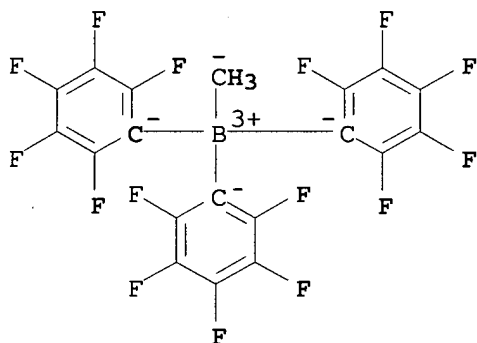
CM 1

CRN 185549-29-5
CMF C17 H18 N Zr
CCI CCS



CM 2

CRN 133445-48-4
 CMF C19 H3 B F15
 CCI CCS



CM 3

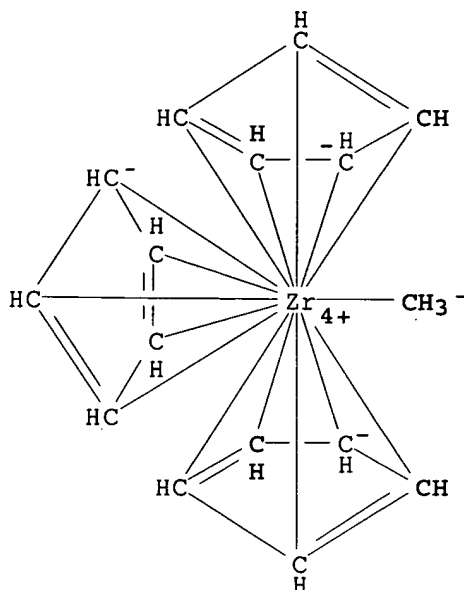
CRN 75-09-2
 CMF C H2 Cl2

Cl-CH₂-Cl

IT 185549-24-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. and structure of tris(cyclopentadienyl)zirconium
 acetonitrile complex)

RN 185549-24-0 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)methyl- (9CI) (CA
 INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

IT 193899-31-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP
 (Preparation)

(crystal structure; prepn. and structure of
 tris(cyclopentadienyl)zirconium acetonitrile complex)

IT 1109-15-5, Tris(pentafluorophenyl)borane 185549-24-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. and structure of tris(cyclopentadienyl)zirconium
 acetonitrile complex)

L31 ANSWER 20 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1997:76759 Document No. 126:89510 Synthesis and Structure of
 Donor-Ligand-Stabilized Tris(cyclopentadienyl)zirconium Cations.
 Brackemeyer, Thomas; Erker, Gerhard; Froehlich, Roland
 (Organisch-Chemisches Institut, Universitaet Muenster, Muenster,
 D-48149, Germany). Organometallics, 16(4), 531-536 (English)
 1997. CODEN: ORGND7. ISSN: 0276-7333. Publisher: American
 Chemical Society.

AB Treatment of $\text{Cp}_2\text{Zr}(\text{Cl})\text{Me}$ (6) with Na cyclopentadienide gives Cp_3ZrMe
 (7). Its reaction with dimethylanilinium tetraphenylborate yields
 the $\text{Cp}_3\text{Zr}(\text{THF})^+$ cation. $[\text{Cp}_3\text{Zr}^+ \text{MeB}(\text{C}_6\text{F}_5)_3^-]$ (9) is generated by
 treatment of 7 with tris(pentafluorophenyl)borate. Nitriles add to
 9 to form the ligand-stabilized tris(η^5 -
 cyclopentadienyl)zirconium cation systems $\text{Cp}_3\text{Zr}(\text{N.tplbond.CR})^+$.
 With tert-Bu isonitrile, 9 is transformed to yield the
 donor-ligand-stabilized $[\text{Cp}_3\text{Zr}(\text{C.tplbond.NCMe}_3)^+ \text{MeB}(\text{C}_6\text{F}_5)_3^-]$ salt
 (12). CO adds to 9 to give the cationic metal carbonyl complex
 $[\text{Cp}_3\text{Zr}(\text{CO})^+ \text{MeB}(\text{C}_6\text{F}_5)_3^-]$ (13). Both cation complexes 12 and 13 were
 characterized by x-ray diffraction.

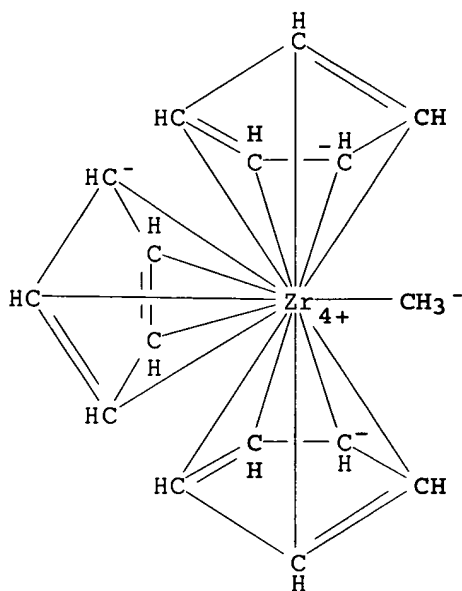
IT 185549-24-0P

RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(crystal structure; prepn., reactions and catalyst for polymn. of ethene)

RN 185549-24-0 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)methyl- (9CI) (CA INDEX NAME)



IT 185549-34-2P 185549-37-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and crystal structure of)

RN 185549-34-2 HCAPLUS

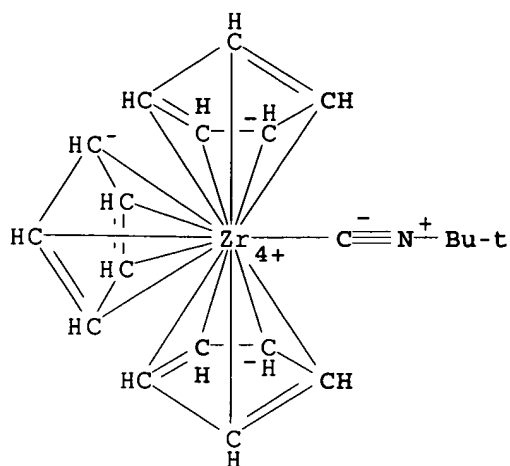
CN Zirconium(1+), tris(η^5 -2,4-cyclopentadien-1-yl) [2-(isocyano- κ C)-2-methylpropane]-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 185549-33-1

CMF C20 H24 N Zr

CCI CCS

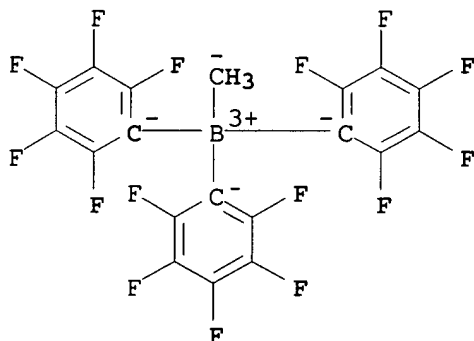


CM 2

CRN 133445-48-4

CMF C19 H3 B F15

CCI CCS



RN 185549-37-5 HCAPLUS

CN Zirconium(1+), carbonyltris(η⁵-2,4-cyclopentadien-1-yl)-, (T-4)-methyltris(pentafluorophenyl)borate(1-), compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 75-09-2

CMF C H2 Cl2

Cl-CH₂-Cl

CM 2

CRN 185549-36-4

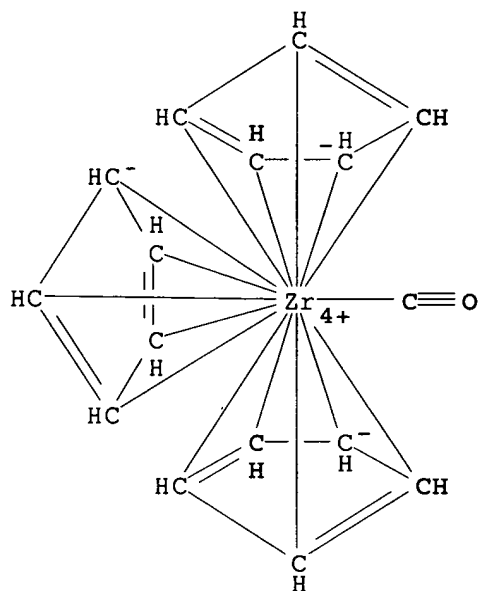
CMF C19 H3 B F15 . C16 H15 O Zr

CM 3

CRN 185549-35-3

CMF C16 H15 O Zr

CCI CCS

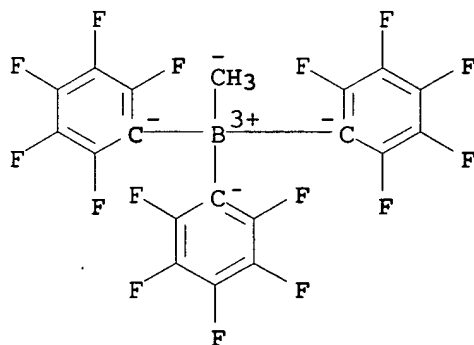


CM 4

CRN 133445-48-4

CMF C19 H3 B F15

CCI CCS



IT 185549-36-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and mol. structure of)

RN 185549-36-4 HCAPLUS

CN Zirconium(1+), carbonyltris(η⁵-2,4-cyclopentadien-1-yl)-,

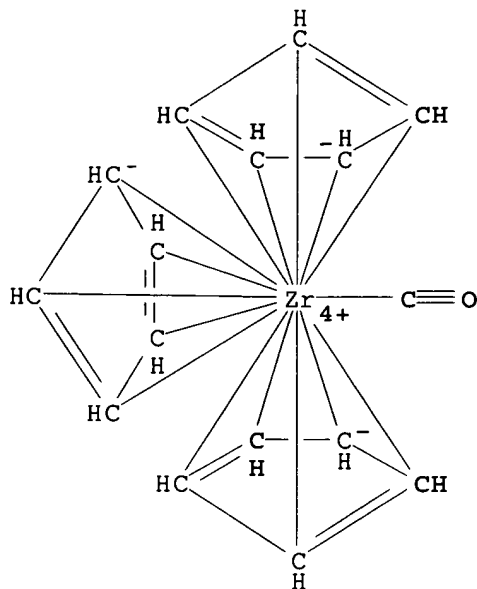
(T-4) -methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 185549-35-3

CMF C16 H15 O Zr

CCI CCS

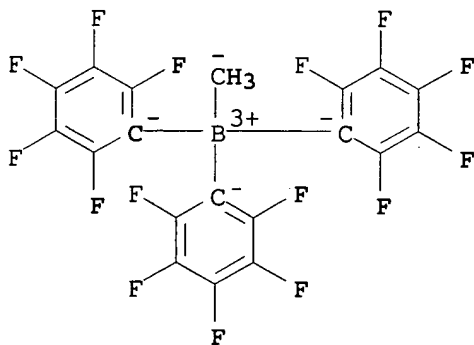


CM 2

CRN 133445-48-4

CMF C19 H3 B F15

CCI CCS



IT 185549-26-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)

(prepn. and reaction with isocyanide)

RN 185549-26-2 HCAPLUS

CN Zirconium(1+), tris(η5-2,4-cyclopentadien-1-yl)-,

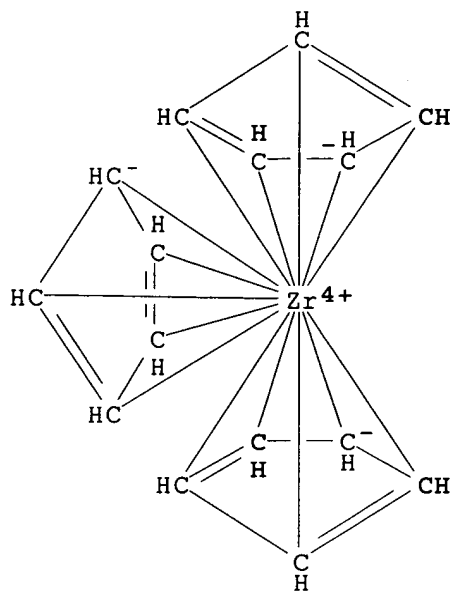
(T-4) -methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 185549-25-1

CMF C15 H15 Zr

CCI CCS

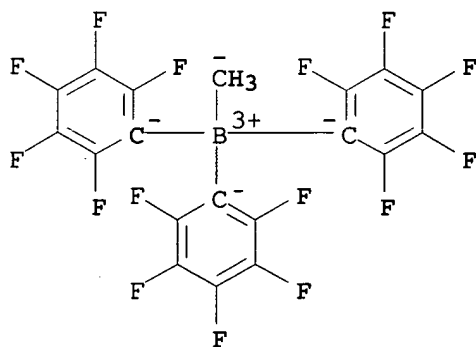


CM 2

CRN 133445-48-4

CMF C19 H3 B F15

CCI CCS



IT 185549-28-4P 185549-30-8P 185549-32-0P

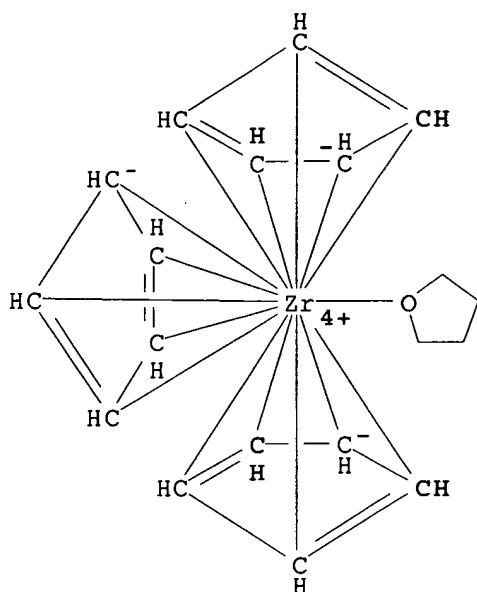
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 185549-28-4 HCAPLUS

CN Zirconium(1+), tris(η5-2,4-cyclopentadien-1-yl)(tetrahydrofuran) -
, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

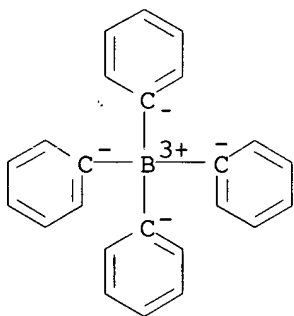
CM 1

CRN 185549-27-3
 CMF C19 H23 O Zr
 CCI CCS



CM 2

CRN 4358-26-3
 CMF C24 H20 B
 CCI CCS

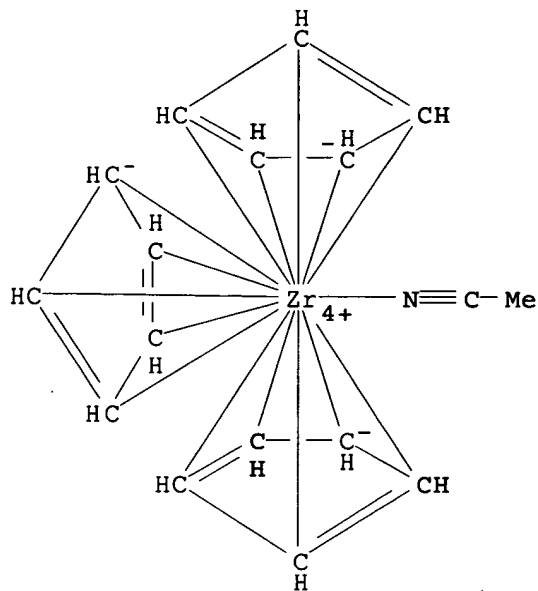


RN 185549-30-8 HCAPLUS
 CN Zirconium(1+), (acetonitrile)tris(η^5 -2,4-cyclopentadien-1-yl)-,
 (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

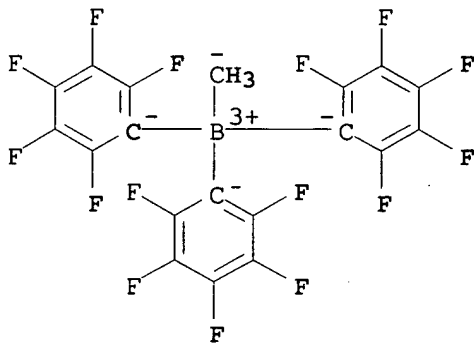
CRN 185549-29-5
 CMF C17 H18 N Zr

CCI CCS



CM 2

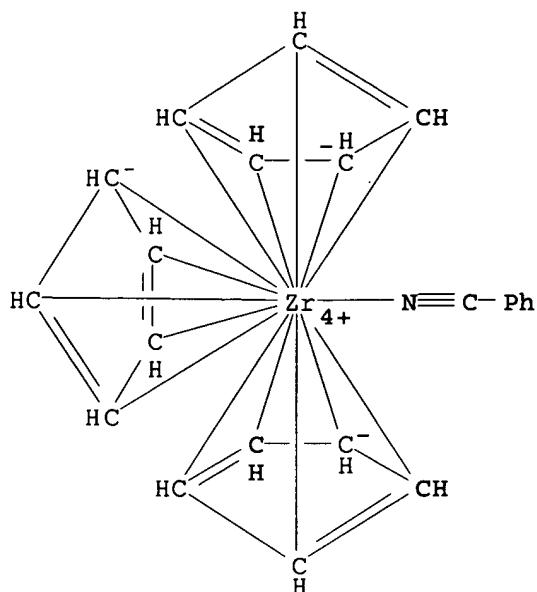
CRN 133445-48-4
 CMF C19 H3 B F15
 CCI CCS



RN 185549-32-0 HCAPLUS
 CN Zirconium(1+), (benzonitrile)tris(η5-2,4-cyclopentadien-1-yl)-,
 (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

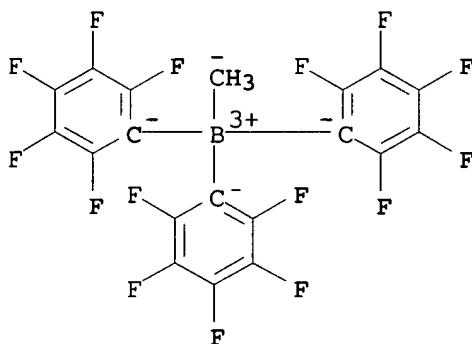
CM 1

CRN 185549-31-9
 CMF C22 H20 N Zr
 CCI CCS



CM 2

CRN 133445-48-4
 CMF C19 H3 B F15
 CCI CCS



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 35, 75

IT 185549-24-0P

RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN
 (Synthetic preparation); PREP (Preparation); RACT (Reactant or
 reagent); USES (Uses)

(crystal structure; prepn., reactions and catalyst for polymn. of
 ethene)

IT 185549-34-2P 185549-37-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP
 (Preparation)

(prepn. and crystal structure of)

IT 185549-36-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP

(Preparation)

(prepn. and mol. structure of)

IT 185549-26-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)

(prepn. and reaction with isocyanide)

IT 185549-28-4P 185549-30-8P 185549-32-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L31 ANSWER 21 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1996:360121 Document No. 125:115214 Synthesis and catalytic properties
of ansa-binuclear metallocenes of the Group IV transition metals.

Ushioda, Tsutomu; Green, Malcolm L. H.; Haggitt, Jane; Yan, Xuefeng
(Inorganic Chemistry Laboratory, South Parks Road, Oxford, OX1 3QR,
UK). Journal of Organometallic Chemistry, 518(1-2), 155-166
(English) 1996. CODEN: JORCAI. ISSN: 0022-328X.

Publisher: Elsevier.

AB The new ansa-bridged mono- and bi-nuclear Group IV metallocenes,

{Zr[X(η -C5H4)2](η -C5H5)Cl} (where, X = SiMe2, CMe2CMe2),
{[(η -C5H5)HfCl2][μ - η -C5H4-(SiMe2)- η -C5H4](η -
C5H5)HfCl2]}, {[(η -C5H5)ZrCl2][μ - η -C5H4-
(SiMe2CH2CH2SiMe2)- η -C5H4](η -C5H5)ZrCl2]},
{[(η -C5H5)ZrCl2][μ - η -C5H4-(SiMe2)- η -C9H6](η -
C5H5)ZrCl2]}, {[(η -C5H5)ZrCl2][μ - η -C9H6-(SiMe2)- η -
C9H6](η -C5H5)ZrCl2]}, {[(η -C5H5)ZrCl2][μ - η -C5H4-
(SiMe2)- η -C5H4](η -C5H5)MCl2]}, M = Hf or Ti,
{[(η -C5H5)ZrCl2][μ - η -C5H4-(SiMe2)- η -C5H4](η -
C5Me5)TiCl2]}, and {[(η -C5H5)ZrCl2][μ - η -C5H4-(SiMe2)-
 η -C5H4][TiCl3]} are described. These compds. in the presence of
methylaluminoxane are catalysts for the polymn. of ethene and
propene.

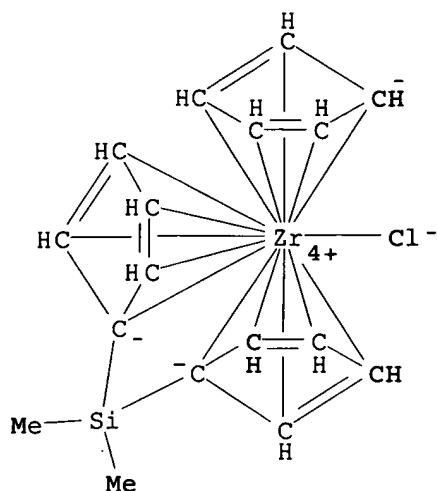
IT 179400-07-8P 179400-08-9P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)

(prepn. and catalytic properties of ansa-binuclear metallocenes
of the Group IV transition metals for polymn. of ethylene and
propylene)

RN 179400-07-8 HCAPLUS

CN Zirconium, chloro(η 5-2,4-cyclopentadien-1-
yl)[(dimethylsilylene)bis(η 5-2,4-cyclopentadien-1-ylidene)]-
(9CI) (CA INDEX NAME)



RN 179400-08-9 HCAPLUS

CN Zirconium, chloro(η^5 -2,4-cyclopentadien-1-yl) [(1,1,2,2-tetramethyl-1,2-ethanediyl)bis(η^5 -2,4-cyclopentadien-1-ylidene)]-(9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 67

IT 144375-09-7P **179400-07-8P 179400-08-9P**

179400-09-0P 179400-10-3P 179400-11-4P 179400-12-5P

179400-13-6P 179400-14-7P 179400-15-8P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. and catalytic properties of ansa-binuclear metallocenes of the Group IV transition metals for polymn. of ethylene and propylene)

L31 ANSWER 22 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1996:188520 Document No. 124:261808 New mono- and bi-nuclear ansa-metallocenes of zirconium and hafnium as catalysts for the polymerization of ethene and propene. Diamond, Gary M.; Chernega, Alexander N.; Mountford, Philip; Green, Malcolm L. H. (Inorganic Chem. Lab., Oxford, OX1 3QR, UK). Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (6), 921-38 (English) 1996. CODEN: JCOTBI. ISSN: 0300-9246. Publisher: Royal Society of Chemistry.

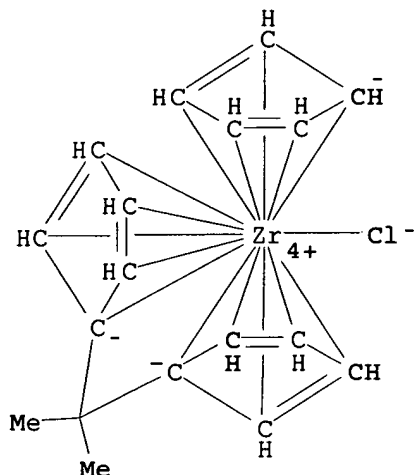
AB The new ansa-metallocenes $[M\{Me_2C(\eta-C_5H_4)(\eta^2-C_9H_6)\}(\eta-C_5H_5)Cl]$ $[M = Zr \text{ (crystal structure) or Hf}]$, $[Zr\{Me_2C(\eta-C_5H_4)(\eta^3-C_{13}H_8)\}(\eta-C_5H_5)Cl]$ (crystal structure), $[X_2(\eta-C_5H_5)M\{C_5H_4(CMe_2)C_9H_6\}M^*(\eta-C_5H_5)X_2]$ $(X = Cl, M, M^* = Zr, Zr; Hf, Hf; Zr, Hf; or Hf, Zr; X = Me, M, M^* = Zr, Zr, Hf; Hf, Zr; or Hf, Hf)$, $[Cl_2(\eta-C_5H_5)Zr\{C_5H_4(CMe_2)C_9H_6\}Zr(\eta-C_5Me_5)Cl_2]$, $[M(C_5H_4)CMe_2(C_9H_7)](\eta-C_5BH_5)Cl_2]$ $(M = Zr \text{ or Hf})$ and $[Zr\{C_5H_4CMe_2(C_9H_7)\}(\eta-C_5H_5)Me_2]$ have been prep'd. and characterized. The activity of the metallocenes as cocatalysts for the polymn. of ethene and propene has been evaluated.

IT 152337-81-0P 152337-82-1P

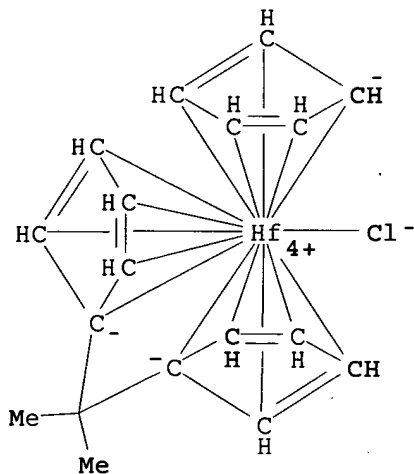
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. and structure and catalytic activity in olefin polymn.)

RN 152337-81-0 HCAPLUS
 CN Zirconium, chloro(η^5 -2,4-cyclopentadien-1-yl) [(1-methylethylidene)bis(η^5 -2,4-cyclopentadien-1-ylidene)]- (9CI)
 (CA INDEX NAME)



RN 152337-82-1 HCAPLUS
 CN Hafnium, chloro(η^5 -2,4-cyclopentadien-1-yl) [(1-methylethylidene)bis(η^5 -2,4-cyclopentadien-1-ylidene)]- (9CI)
 (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 29, 75

IT 152337-81-0P 152337-82-1P 153882-72-5P
 154647-67-3P 154647-68-4P 154647-69-5P 154647-71-9P
 154647-72-0P 155890-64-5P 155890-65-6P 155890-66-7P
 155890-67-8P 155890-68-9P 175666-63-4P 175666-64-5P
 175666-65-6P 175666-66-7P 175666-67-8P 175666-68-9P

RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. and structure and catalytic activity in olefin polymn.)

L31 ANSWER 23 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
 1995:643097 Document No. 123:112266 Synthesis, Structure, and
 Reactions of $(\eta^5\text{-C}_5\text{H}_5)_3\text{Zr}$. Lukens, Wayne W. ,Jr.; Andersen,
 Richard A. (Lawrence Berkeley Laboratory, University of California,
 Berkeley, CA, 94720, USA). Organometallics, 14(7), 3435-9 (English)
 1995. CODEN: ORGND7. ISSN: 0276-7333. OTHER SOURCES:

CASREACT 123:112266. Publisher: American Chemical Society.

AB Cp_3Zr was synthesized by the redn. of Cp_4Zr ($\text{Cp} = \text{C}_5\text{H}_5$). Cp_3Zr is
 monomeric in the solid state by x-ray diffraction with three Cp
 rings bonded to Zr in an η^5 fashion. The 19-electron
 metallocene has a single unpaired electron and an axial EPR spectrum
 in frozen soln. It does not appear to form base adducts but does
 react by atom abstraction. The obsd. spectra and reactions are
 explained using the MO model for Cp_3M developed by Bursten and
 Strittmatter and previously by Lauher and Hoffmann.

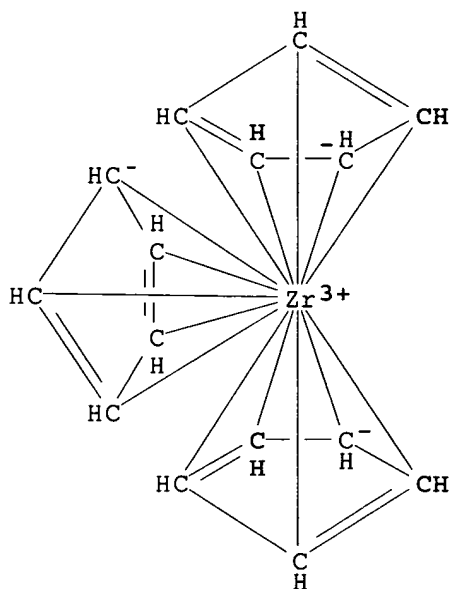
IT 131323-29-0P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)

(crystal structure; prepn., structure, and reactions of
 tris(cyclopentadienyl)zirconium)

RN 131323-29-0 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX
 NAME)



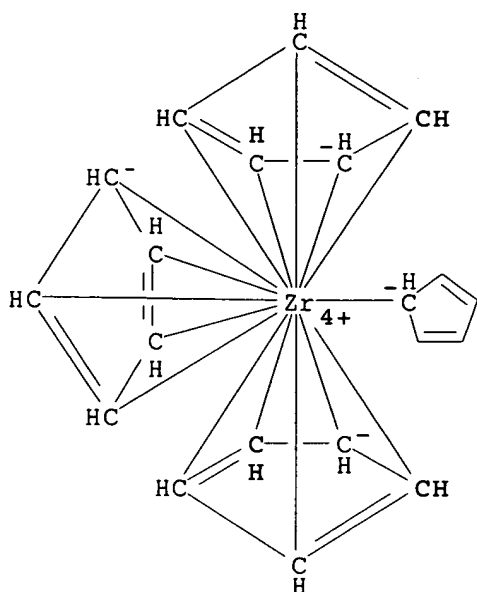
IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium

RL: RCT (Reactant); RACT (Reactant or reagent)

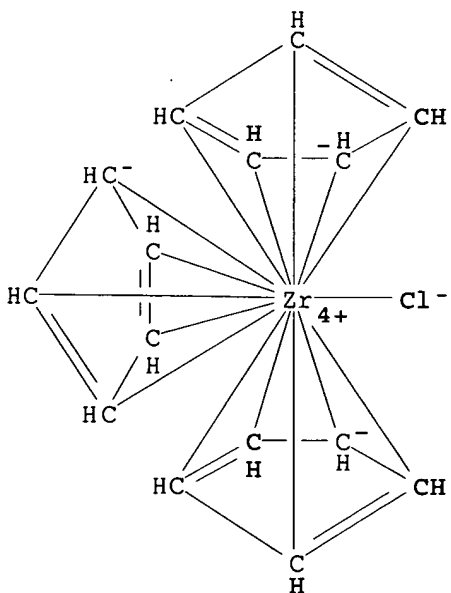
(prepn., structure, and reactions of
 tris(cyclopentadienyl)zirconium)

RN 1273-01-4 HCAPLUS

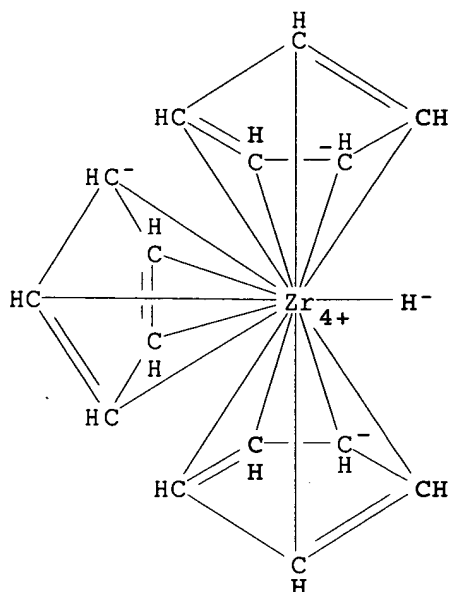
CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-
 yl- (9CI) (CA INDEX NAME)



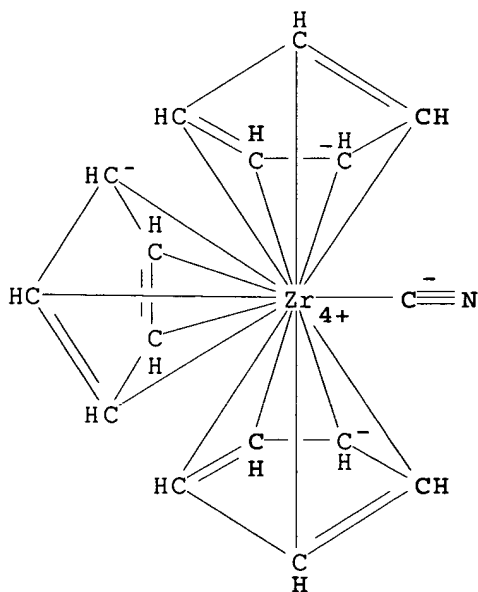
IT 62343-37-7P 78446-26-1P,
 Tris(cyclopentadienyl)zirconium hydride 165966-21-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn., structure, and reactions of
 tris(cyclopentadienyl)zirconium)
 RN 62343-37-7 HCAPLUS
 CN Zirconium, chlorotris(η^5 -2,4-cyclopentadien-1-yl) - (9CI) (CA
 INDEX NAME)



RN 78446-26-1 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)hydro- (9CI) (CA
 INDEX NAME)

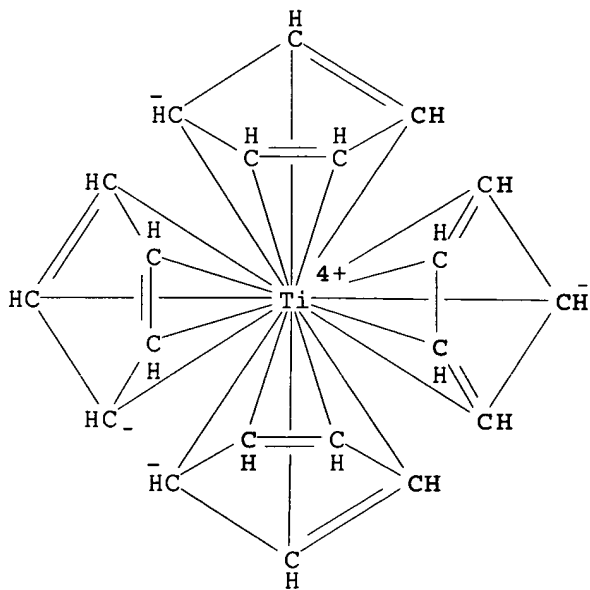


RN 165966-21-2 HCAPLUS
 CN Zirconium, (cyano-C)tris(η5-2,4-cyclopentadien-1-yl)- (9CI) (CA
 INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75
 IT 131323-29-0P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (crystal structure; prepn., structure, and reactions of
 tris(cyclopentadienyl)zirconium)

- IT 1005-93-2, Trimethylolpropane phosphate 1273-01-4,
Tetrakis(cyclopentadienyl)zirconium 12081-88-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn., structure, and reactions of
tris(cyclopentadienyl)zirconium)
- IT 62343-37-7P 70693-90-2P 78446-26-1P,
Tris(cyclopentadienyl)zirconium hydride 165966-21-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., structure, and reactions of
tris(cyclopentadienyl)zirconium)
- L31 ANSWER 24 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
1994:567561 Document No. 121:167561 Manufacture of titanium-containing
thin film by chemical vapor deposition. Sekiguchi, Atsushi; Tobe,
Akina (Anelva Corp, Japan). Jpn. Kokai Tokkyo Koho JP 06158321 A2
19940607 Heisei, 7 pp. (Japanese). CODEN: JKXXAF.
APPLICATION: JP 1992-334888 19921124.
- AB The title method involves setting a substrate in a reactor,
evacuating the reactor, vaporizing tris(cyclopentadienyl)titanium
and/or tetra(cyclopentadienyl)titanium, introducing the compd. into
the reactor, and reacting the compd. near the substrate to deposit a
Ti-contg. thin film. A Ti film with good step coverage was obtained
at low temp.
- IT 11079-32-6, Tetra(cyclopentadienyl)titanium
RL: PROC (Process)
(CVD of titanium-contg. thin film from, with good step coverage)
- RN 11079-32-6 HCAPLUS
CN Titanium, tetrakis(η^5 -2,4-cyclopentadien-1-yl) - (9CI) (CA INDEX
NAME)



- IC ICM C23C016-18
ICS C23C016-34; C23C016-42; H01L021-205; H01L021-285
- CC 75-1 (Crystallography and Liquid Crystals)
Section cross-reference(s): 29
- IT 11079-32-6, Tetra(cyclopentadienyl)titanium 52700-41-1,
Tris(cyclopentadienyl)titanium

RL: PROC (Process)

(CVD of titanium-contg. thin film from, with good step coverage)

L31 ANSWER 25 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1994:270662 Document No. 120:270662 Contributions to the chemistry of phosphorus. 227. HP4- as a complex ligand: Formation and properties of $[(\eta^5\text{-C}_5\text{H}_5)_2\text{ZrCl}(\text{P}_4\text{H})]$, $[(\eta^5\text{-C}_5\text{Me}_5)_2\text{ZrCl}(\text{P}_4\text{H})]$, and $[(\eta^5\text{-C}_5\text{H}_5)_3\text{Zr}(\text{P}_4\text{H})]$. Baudler, M.; Wingert, B. (Inst. Anorg. Chem., Univ. Koeln, Cologne, Germany). Zeitschrift fuer Anorganische und Allgemeine Chemie, 619(12), 1977-83 (German) 1993. CODEN: ZAACAB. ISSN: 0044-2313. OTHER SOURCES: CASREACT 120:270662.

AB The novel complexes $[(\eta^5\text{-C}_5\text{H}_5)_2\text{ZrCl}(\text{P}_4\text{H})]$ (1), $[(\eta^5\text{-C}_5\text{Me}_5)_2\text{ZrCl}(\text{P}_4\text{H})]$ (2), and $[(\eta^5\text{-C}_5\text{H}_5)_3\text{Zr}(\text{P}_4\text{H})]$ (3) were prep'd. by the reaction of a soln. of (Na/K)HP4 with the zirconocene derivs. $[(\eta^5\text{-C}_5\text{H}_5)_2\text{ZrCl}_2]$, $[(\eta^5\text{-C}_5\text{Me}_5)_2\text{ZrCl}_2]$, and $[(\eta^5\text{-C}_5\text{H}_5)_3(\eta^1\text{-C}_5\text{H}_5)\text{Zr}]$ under suitable conditions. The structure of the compds. 1-3, which are only stable in soln., has been elucidated by means of ^{31}P -NMR spectroscopy. It is highly probable that the exo,endo isomer exists in each case. In addn., further isomers of lower relative abundances have been obsd., in which the ligands presumably exhibit a different spatial orientation relatively to each other.

IT 154797-51-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 154797-51-0 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)(tetraphosphabicyclo[1.1.0]butanato-P2)- (9CI) (CA INDEX NAME)

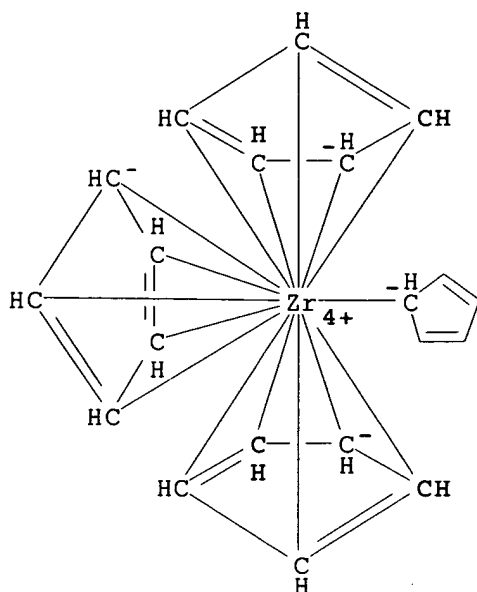
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydridobicyclotetraphosphide anion)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 154797-49-6P 154797-50-9P **154797-51-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

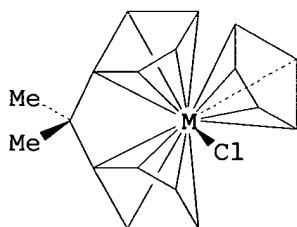
IT **1273-01-4** 1291-32-3, Zirconocene dichloride 54039-38-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydridobicyclotetraphosphide anion)

L31 ANSWER 26 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1994:77404 Document No. 120:77404 ansa-Bridged tris(cyclopentadienyl) compounds of zirconium and hafnium: x-ray crystal structures of $[M[Me_2C(\eta^5-C_5H_4)_2][\eta^5-C_5H_5)Cl]$ ($M = Zr$ or Hf). Diamond, Gary M.; Green, Malcolm L. H.; Popham, Neil A.; Chernega, Alexander N. (Inorg. Chem. Lab., Oxford, OX1 3QR, UK). Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (16), 2535-6 (English) **1993**. CODEN: JCDTBI. ISSN: 0300-9246. OTHER SOURCES: CASREACT 120:77404.

GI



I

AB Reaction of $Li_2[Me_2C(C_5H_4)_2]$ with $[Zr(\eta^5-C_5H_5)Cl_3]$.DME and $[Hf(\eta^5-C_5H_5)Cl_3]$.2THF in PhMe gave 41-43% new ansa-bridged title compds. I ($M = Zr, Hf$), resp., which were characterized by x-ray crystallog. The latter is the 1st example of a tris(η^5 -cyclopentadienyl) deriv. of hafnium.

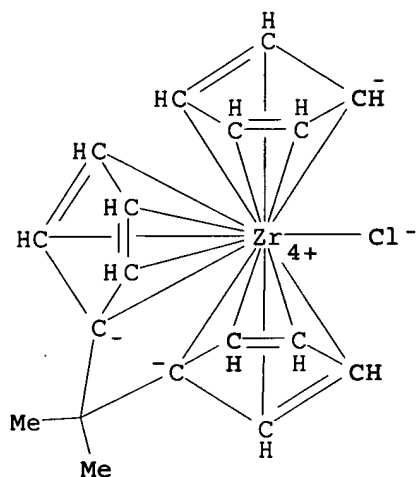
IT 152337-81-0P 152337-82-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and crystal and mol. structure of)

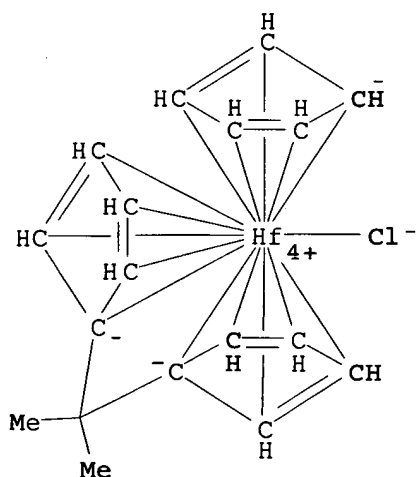
RN 152337-81-0 HCAPLUS

CN Zirconium, chloro(η^5 -2,4-cyclopentadien-1-yl)[(1-methylethylidene)bis(η^5 -2,4-cyclopentadien-1-ylidene)]- (9CI)
(CA INDEX NAME)



RN 152337-82-1 HCAPLUS

CN Hafnium, chloro(η^5 -2,4-cyclopentadien-1-yl)[(1-methylethylidene)bis(η^5 -2,4-cyclopentadien-1-ylidene)]- (9CI)
(CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75

IT 152337-81-0P 152337-82-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and crystal and mol. structure of)

L31 ANSWER 27 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1993:449516 Document No. 119:49516 Mass-spectrometric studies of some new hafnocene dialcoholates. Grafov, A. V.; Favretto, Donata; Traldi, Pietro; Battiston, Giovanni A.; Porchia, Marina; Rossetto, Gilberto; Zanella, Pierino (Inst. Gen. Inorg. Chem., Kiev, Ukraine). Rapid Communications in Mass Spectrometry, 7(2), 158-62 (English) 1993. CODEN: RCMSEF. ISSN: 0951-4198.

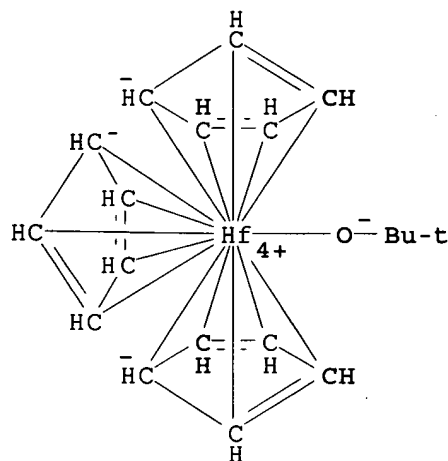
AB The electron ionization mass spectrometric behavior of a new class of hafnocene dialcoholates, e.g., CpHf(endo-NBL)₂ [endo-HNBL = (+)-endo-norborneol] and, for comparison, of hafnocene dichloride, is discussed. They are also compared on the basis of mass-analyzed ion kinetic energy spectrometry. Fragmentation patterns of oxygen-contg. species give relevant information on their potential as precursors for the deposition of HfO₂ thin films via metal-org. chem. vapor deposition.

IT 148448-31-1

RL: PRP (Properties)
(mass spectra of)

RN 148448-31-1 HCAPLUS

CN Hafnium, tris(η⁵-2,4-cyclopentadien-1-yl) (2-methyl-2-propanolato) - (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 73

IT 12116-66-4 148448-29-7 148448-30-0 148448-31-1
148554-44-3

RL: PRP (Properties)
(mass spectra of)

L31 ANSWER 28 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1993:14775 Document No. 118:14775 A solution-state dipole moment and microwave dielectric loss study of titanium, zirconium, hafnium and tin cyclopentadienyl compounds. Allen, Gregory W.; Aroney, Manuel J.; Filipczuk, Stephen W.; Phillips, Leonidas (Dep. Inorg. Chem., Univ. Sydney, Sydney, 2006, Australia). Journal of Molecular Liquids, 54(1-3), 147-54 (English) 1992. CODEN: JMLIDT. ISSN: 0167-7322.

AB Dielec. properties of cyclopentadienyl complexes Cp₂MX₂ and Cp₄M (M = Ti, Zr, Hf or Sn; X = Cl or Br; Cp = cyclopentadienyl) have been

investigated in dil. benzene or 1,4-dioxane soln. using the std. refractivity and microwave dielec. absorption techniques. The highly dipolar nature of the mols. Cp_2MX_2 has been confirmed for the soln.-state and it has been shown that at. distortion polarizations for these compds. are small. The dielec. relaxation times for the Cp_2MX_2 and Cp_4Hf are also highly dipolar indicating nonequiv. Cp rings about the metal. The predominant component of dielec. relaxation for these is by mol. tumbling although weakly absorbing intramol. modes must also exist. The complex Cp_4Sn has a low dipole moment and is weakly absorbing, this being consistent with a $(\eta^1\text{-Cp})_4\text{Sn}$ structure.

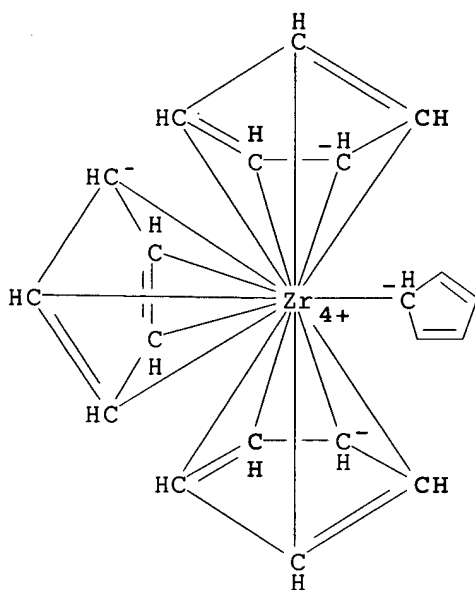
IT 1273-01-4

RL: PRP (Properties)

(elec. dipole moment of, in benzene or dioxane soln.)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 76-9 (Electric Phenomena)

Section cross-reference(s): 29

IT 1271-19-8 1273-01-4 1291-32-3 1293-73-8 1294-67-3

3559-76-0 12116-66-4 12149-28-9 37260-83-6

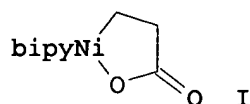
RL: PRP (Properties)

(elec. dipole moment of, in benzene or dioxane soln.)

L31 ANSWER 29 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1992:447542 Document No. 117:47542 Nickelalactones as synthetic building blocks. Sonochemical and bimetal activation in cross coupling reaction with alkyl halides. Fischer, Reinald; Walther, Dirk; Braeunlich, Gabriele; Undeutsch, Bernd; Ludwig, Werner; Bandmann, Heinz (Chem. Fak., Friedrich-Schiller-Univ., Jena, O-6900, Germany). Journal of Organometallic Chemistry, 427(3), 395-407 (German) 1992. CODEN: JORCAI. ISSN: 0022-328X. OTHER SOURCES: CASREACT 117:47542.

GI



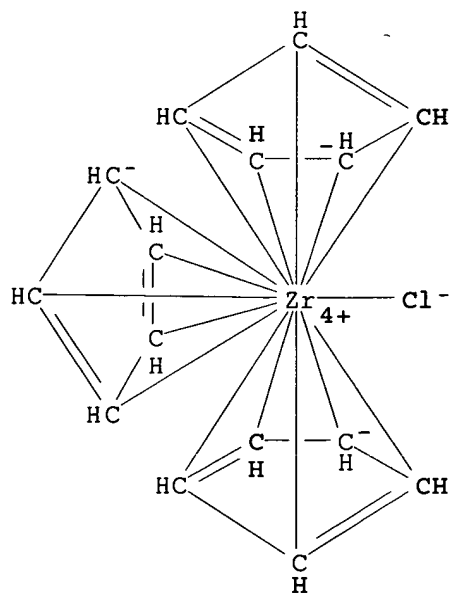
AB Nickelalactones with five- (e.g. I, bipy = 2,2'-bipyridine) and six-membered chelate ring structures can be synthesized in a simple one-pot reaction, starting from Ni(acac)₂, bipy, Et₃Al and cyclic anhydrides. In the presence of MnI₂ and by activation with ultrasound, they react selectively with alkyl iodides in cross coupling reactions. E.g., I and cyclohexyl iodide gave 80% cyclohexanepropionic acid. The activating effect of MnI₂ is due to the formation of bimetallic complexes. Many reactive functional groups (e.g., COOR, CHO, CN) can be tolerated. The cross coupling reaction is of preparative value in the synthesis of functionalized carboxylic acids.

IT 62343-37-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(cross coupling of nickelalactone with cyclohexyl iodide in presence of)

RN 62343-37-7 HCAPLUS

CN Zirconium, chlorotris(η⁵-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 29

IT 7790-33-2, Manganese diiodide 10139-47-6, Zinc iodide

10377-58-9, Magnesium iodide 62343-37-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(cross coupling of nickelalactone with cyclohexyl iodide in presence of)

L31 ANSWER 30 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1992:408684 Document No. 117:8684 Catalysts for preparation of polyolefins. Tajima, Yoshio; Nomiyama, Kazutoshi; Kataoka, Naoki; Matsuura, Kazuo (Nippon Oil Co., Ltd., Japan). Eur. Pat. Appl. EP 474391 A2 19920311, 19 pp. DESIGNATED STATES: R: DE, GB. (English). CODEN: EPXXDW. APPLICATION: EP 1991-307633 19910819. PRIORITY: JP 1990-219769 19900821; JP 1990-226955 19900829.

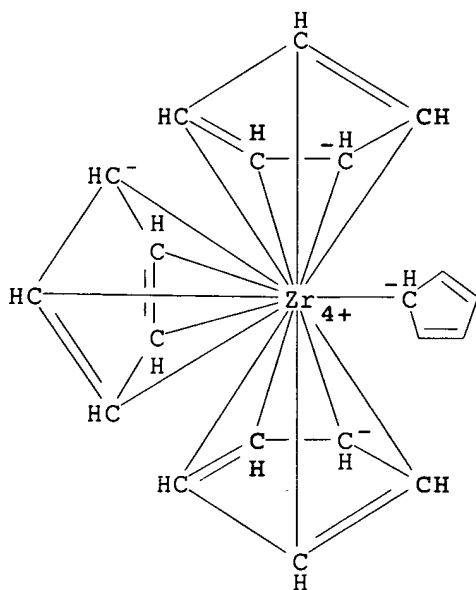
AB Olefins are polymd. in the presence of a catalyst comprising a component obtained by reacting an organoaluminum compd. with water and having ≥ 1 Al-O-Al bond and a solid component obtained by mutual contact of a porous inorg. oxide, a compd. $(RO)_nAlX_{3-n}$ ($R = C1-24$ hydrocarbyl; $X = \text{halo}$; $0 < n \leq 3$), and a compd. R_1pMX_1r [$M = \text{group IVB metal}$; $R_1 = (\text{substituted}) \text{ cyclopentadienyl}, (\text{substituted}) \text{ indenyl}, C7-24 \text{ aralkyl}$; $X = \text{halo}, H, C1-24 \text{ hydrocarbyl}$; $2 \leq p \leq 4$; $0 \leq r \leq 2$; $p + r = 4$], giving polyolefin powders having high bulk d. and satisfactory particle shape. Ethylene and 1-butene were copolymd. in the presence of Me aluminoxane and a solid component prepd. from silica, $(\text{iso-PrO})_3Al$, and bis(cyclopentadienyl)dichlorotitanium.

IT 1273-01-4, Tetracyclopentadienylzirconium 11079-32-6
, Tetracyclopentadienyltitanium

RL: CAT (Catalyst use); USES (Uses)
(catalysts, for polymn. of olefins)

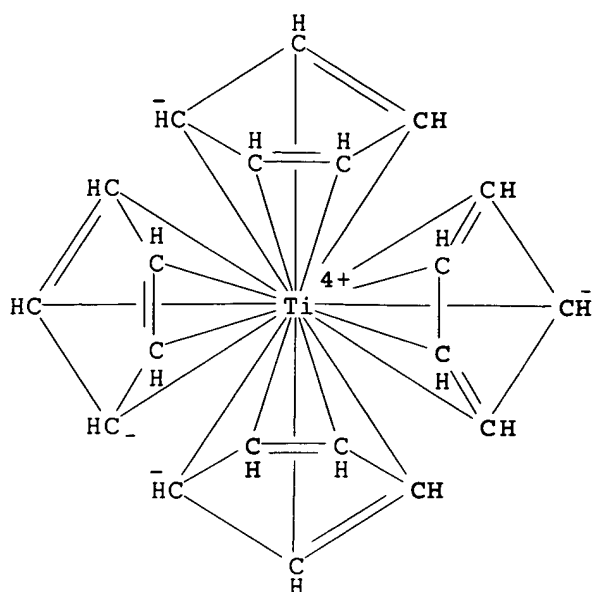
RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



RN 11079-32-6 HCAPLUS

CN Titanium, tetrakis(η^5 -2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



IC ICM C08F004-642

ICS C08F010-00

CC 35-3 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 67

IT 555-31-7, Triisopropoxyaluminum 555-75-9, Triethoxyaluminum
 865-31-6, Trimethoxyaluminum 1271-19-8,
 Bis(cyclopentadienyl)dichlorotitanium 1271-66-5,
 Bis(cyclopentadienyl)dimethyltitanium 1273-01-4,
 Tetracyclopentadienylzirconium 1273-09-2,
 Bis(cyclopentadienyl)diphenyltitanium 1278-83-7 1291-32-3,
 Bis(cyclopentadienyl)dichlorozirconium 1291-45-8 2092-14-0
 2269-22-9, Tri-sec-butoxyaluminum 3085-29-8 3085-30-1,
 Tributoxyaluminum 3314-55-4 3314-57-6, Butoxydichloroaluminum
 10092-89-4 11079-32-6, Tetracyclopentadienyltitanium
 11087-28-8 11087-33-5 12109-84-1 12113-02-9 12116-66-4
 12129-76-9 12148-49-1 12636-72-5, Bis(cyclopentadienyl)dimethylz
 irconium 12715-66-1 14814-04-1 15086-27-8, Triphenoxyaluminum
 17520-19-3, Tetrabenzyltitanium 22005-08-9 23970-94-7
 24356-01-2, Tetrabenzylzirconium 24449-02-3 27177-69-1
 32838-37-2 33715-52-5 36945-13-8, Tetraneopentyltitanium
 37260-88-1, Bis(cyclopentadienyl)dimethylhafnium 38010-72-9,
 Tetraneopentylzirconium 39333-72-7 41826-69-1 41996-90-1
 49596-02-3 49596-04-5 50654-35-8 51177-89-0 51231-81-3
 56770-59-3 62652-01-1 63817-87-8 68193-38-4 69124-52-3
 75061-73-3 78169-38-7, Bis(methylcyclopentadienyl)dimethyltitanium
 84501-84-8 91454-53-4 100080-82-8 109086-38-6 109550-91-6
 110487-85-9 110567-61-8 112243-79-5 112531-75-6 112531-76-7
 130139-66-1 135910-63-3 141752-67-2 141752-68-3 141778-08-7
 141778-09-8 141778-10-1 141801-10-7 141993-45-5 141993-46-6

RL: CAT (Catalyst use); USES (Uses)

(catalysts, for polymn. of olefins)

L31 ANSWER 31 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1991:43011 Document No. 114:43011 Bonding in tris(η⁵-cyclopentadienyl) actinide complexes. 5. A comparison of the bonding in neptunium, plutonium, and transplutonium compounds with

that in lanthanide compounds and a transition-metal analog.
 Strittmatter, Richard J.; Bursten, Bruce E. (Dep. Chem., Ohio State Univ., Columbus, OH, 43210, USA). Journal of the American Chemical Society, 113(2), 552-9 (English) 1991. CODEN: JACSAT.
 ISSN: 0002-7863.

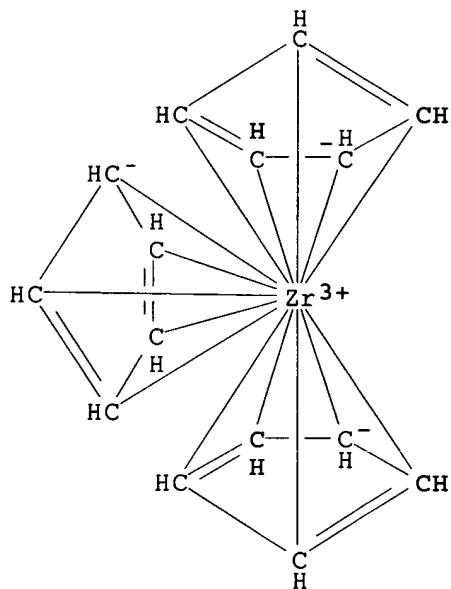
AB Cp3M (M = U, Np, Pu, Am, Cm, Bk, Cf; Cp = η^5 -cyclopentadienyl) were investigated via X α -SW MO calcns. with quasi-relativistic corrections. The 5f-orbital energy drops across the series while the 6d-orbital energy rises. Due to the greater radial extension of the 6d orbitals, the metal 6d orbitals are more important in bonding the Cp ligands than the 5f orbitals. Comparison of the actinide compds. with the lanthanide series reveals some minor differences. The 4f orbitals and 6s orbital of the lanthanides are not as effective at bonding the Cp ligands as the 5f orbitals and 7s orbital of the actinides. Also the "semicore" 5p orbitals of the lanthanides have a greater antibonding influence on the Cp ligands than do the 6p orbitals of the actinides. Comparison of the actinide compds. with (η^5 -Cp)3Zr shows some major differences. The 4d orbitals of zirconium are much more effective at bonding the Cp ligands than the 6d orbitals of the actinides.

IT 131323-29-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (bonding in, quantum-chem. X α -SW calcns. in relation to)

RN 131323-29-0 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

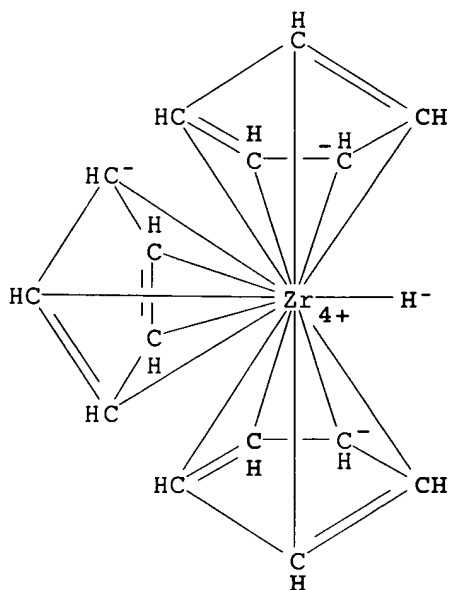
Section cross-reference(s): 22

IT 1272-21-5 1273-98-9 1295-18-7 1298-53-9 1298-55-1
 11077-59-1 12088-04-9 12216-08-9 54007-00-0 63757-59-5
 66969-49-1 127037-41-6 131323-28-9 131323-29-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (bonding in, quantum-chem. X α -SW calcns. in relation to)

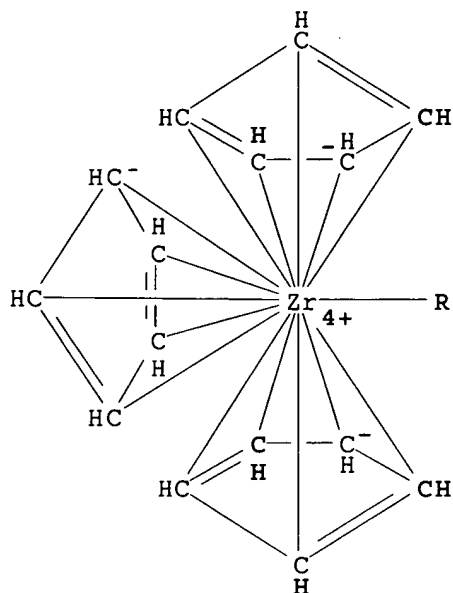
L31 ANSWER 32 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

- 1990:424097 Document No. 113:24097 Some properties of cyclopentadienylzirconium hydride complexes. Strunkina, L. I.; Minacheva, M. Kh.; Klemenkova, Z. S.; Vinogradova, L. V.; Lokshin, B. V. (Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR). Metalloorganicheskaya Khimiya, 2(5), 1054-60 (Russian) 1989 . CODEN: MEKHEX. ISSN: 0235-0114.
- AB Reaction of Cp_2ZrH_2 ($\text{Cp} = \eta^5\text{-cyclopentadienyl}$) with Cp_2ZrBr_2 in THF gave 31% hydride Cp_2ZrBrH (I). Reactions of I and of hydrides $\text{CpZr(L)}_2\text{H}$ [$\text{L} = \text{acetylacetonato}$ (II), $\text{dibenzoylmethanato}$ (III)] and Cp_3ZrH with H_2O , β -diketones, and HCl are reported. E.g., reactions of II with $(\text{PhCO})_2\text{CH}_2$ or of III with $(\text{MeCO})_2\text{CH}_2$ both gave $[(\text{PhCO})_2\text{CH}]_2\text{Zr}[\text{CH}(\text{COMe})_2]_2$. In soln., II, III, and $\text{CpZr(L)}_2\text{Cl}$ are proposed to exist in cis and trans isomers.
- IT 78446-26-1
 RL: RCT (Reactant); RACT (Reactant or reagent) (oxidn. of)
- RN 78446-26-1 HCAPLUS
- CN Zirconium, tris($\eta^5\text{-2,4-cyclopentadien-1-yl}$)hydro- (9CI) (CA INDEX NAME)

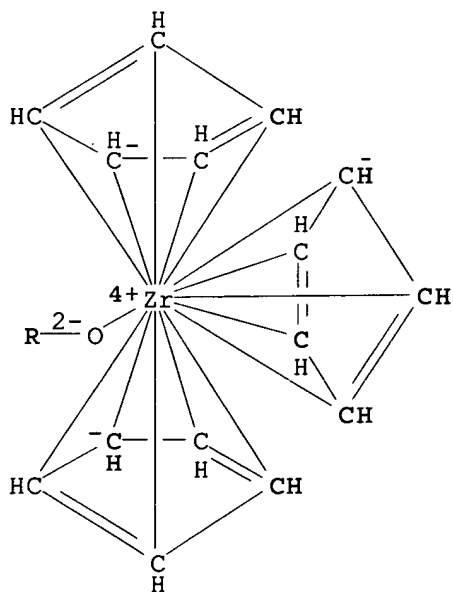


- IT 127713-99-9P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
- RN 127713-99-9 HCAPLUS
- CN Zirconium, hexakis($\eta^5\text{-2,4-cyclopentadien-1-yl}$)- μ -oxodi- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 78446-26-1

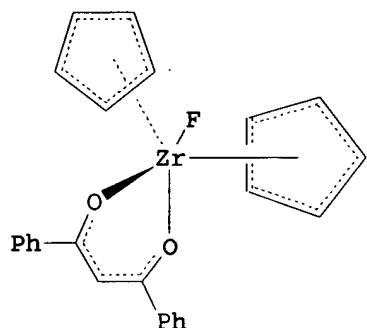
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. of)

IT	12104-61-9P	17217-93-5P	18717-38-9P	35194-88-8P	41654-86-8P
	50803-55-9P	69137-97-9P	73655-98-8P	127713-40-0P	

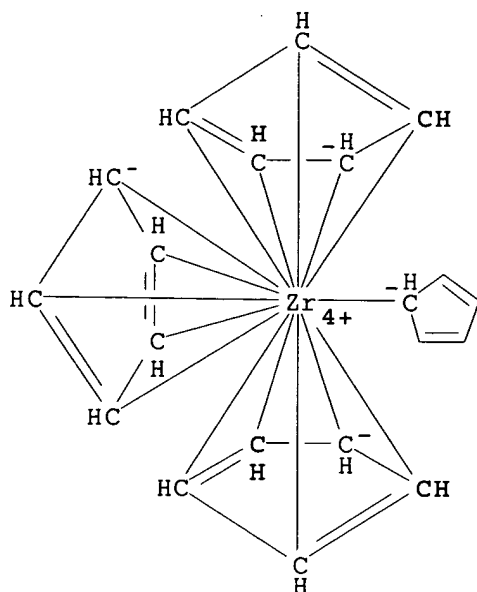
127713-43-3P 127713-99-9P 127759-78-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L31 ANSWER 33 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
1990:139275 Document No. 112:139275 Hydroxides and fluorides of
cyclopentadienylhafnium and -zirconium complexes. Minacheva, M.
Kh.; Dostovalova, V. I.; Klemenkova, Z. S.; Mikhailova, O. A.;
Brainina, E. M.; Lokshin, B. V. (Inst. Elementoorg. Soedin. im.
Nesmeyanova, Moscow, USSR). Metalloorganicheskaya Khimiya, 2(3),
647-53 (Russian) 1989. CODEN: MEKHEX. ISSN: 0235-0114.

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AB Reactions of Cp_2MCl_2 ($\text{Cp} = \eta^5\text{-cyclopentadienyl}$; $\text{M} = \text{Hf}, \text{Zr}$),
[Cp_2MF] 2O , or Cp_4M (same M) with H_2O , HF , and $(\text{PhCO})_2\text{CH}_2$ (bzbzH)
under comparable conditions to give the title complexes were examd.
Treating [Cp_2ZrF] 2O with bzbzH gave pentacoordinate compd.
 $\text{Cp}_2\text{ZrF}(\text{bzbz})$, which was isolated as a single, cis isomer (I).
IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydrogen fluoride)
RN 1273-01-4 HCAPLUS
CN Zirconium, tris($\eta^5\text{-2,4-cyclopentadien-1-yl}$)-2,4-cyclopentadien-1-
yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT **1273-01-4**, Tetrakis(cyclopentadienyl)zirconium 12149-28-9,
Tetrakis(cyclopentadienyl)hafnium

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydrogen fluoride)

L31 ANSWER 34 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1990:55102 Document No. 112:55102 Zirconocene hydrides as reducing
agents of alkylaromatic chloro derivatives and of chlorobenzene.

Strunkina, L. I.; Brainina, E. M.; Minacheva, M. Kh. (Inst.

Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR).

Metalloorganicheskaya Khimiya, 2(3), 677-9 (Russian) **1989**.

CODEN: MEKHEX. ISSN: 0235-0114.

AB Cp₃ZrH (I, Cp = cyclopentadienyl), Cp₂ZrHCl, and Cp₂ZrH₂ (II)

reduced PhCCl₃ to PhCHCl₂, PhCHCl₂ to PhCH₂Cl, and PhCH₂Cl to PhMe.

I and II also reduced PhCl to benzene.

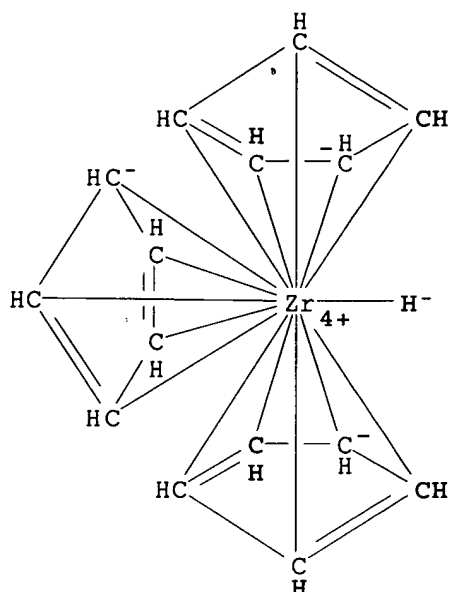
IT **78446-26-1**

RL: RCT (Reactant); RACT (Reactant or reagent)

(reductive dechlorination by, of chlorobenzene and
(chloromethyl)benzenes)

RN 78446-26-1 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)hydro- (9CI) (CA
INDEX NAME)



CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 37342-98-6 **78446-26-1**

RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive dechlorination by, of chlorobenzene and
(chloromethyl)benzenes)

L31 ANSWER 35 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1989:515423 Document No. 111:115423 A molecular orbital study of conformational preferences of the cyclopentadienyl ligand in titanium(IV) and titanium(III) complexes. Hansen, Lillian M.; Marynick, Dennis S. (Dep. Chem., Univ. Texas, Arlington, TX, 76019, USA). Organometallics, 8(9), 2173-9 (English) 1989. CODEN: ORGND7. ISSN: 0276-7333.

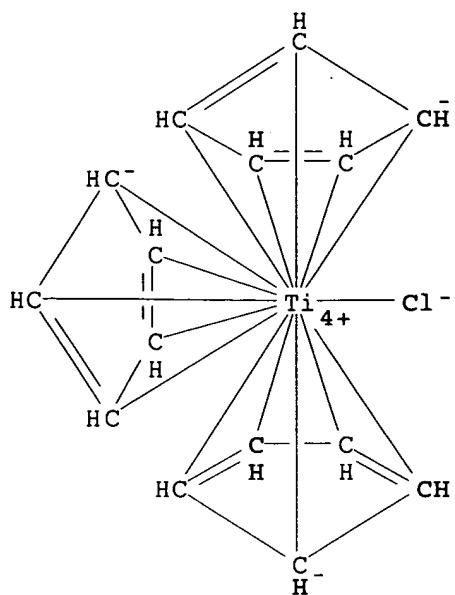
AB A theor. study of the conformational preferences of the cyclopentadienyl (Cp) ligand in titanium(IV) and titanium(III) systems is presented. The method of Partial Retention of Diat. Differential Overlap is used to optimize the geometries of Cl3CpTi, Cl2Cp2Ti, ClCp3Ti, Cp4Ti, and Cp3Ti. The relative stability of structures exhibiting alternative coordination modes of the cyclopentadienyl ligand (η_1 , η_2 , and η_5) was estd. at the ab initio level with an expanded basis set, in some cases including MP2 correlation corrections. From this study, it was detd. that the ground-state conformations of (cyclopentadienyl)titanium(IV) and -titanium(III) complexes are predominantly influenced by electronic factors. A detailed bonding anal. of the unusual η_2 coordination in tris(cyclopentadienyl)titanium(III) indicates that the η_2 conformation is stabilized by π -donating substituents on the nonbonding carbons. A simple localized bonding description of the η_2 -bound ligand is presented, as well as suggestions for further stabilizing this unusual coordination.

IT 11079-20-2 11079-32-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(partial retention of diat. differential overlap MO calcns. of,
conformation in relation to)

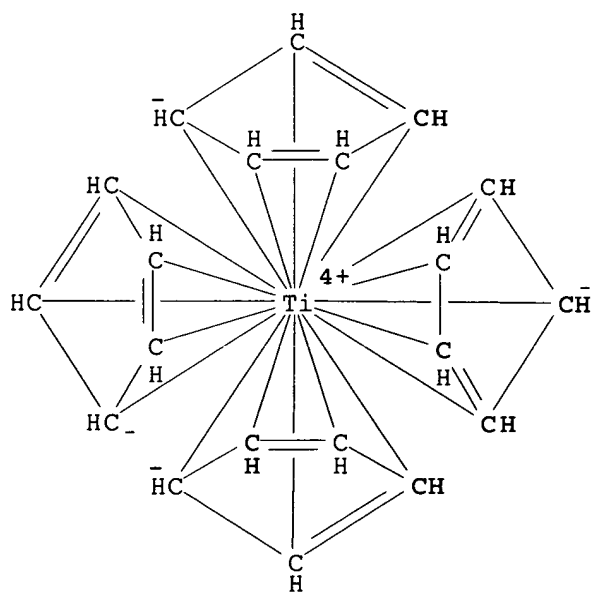
RN 11079-20-2 HCAPLUS

CN Titanium, chlorotris(η^5 -2,4-cyclopentadien-1-yl) - (9CI) (CA INDEX NAME)



RN 11079-32-6 HCAPLUS

CN Titanium, tetrakis(η^5 -2,4-cyclopentadien-1-yl) - (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

IT 1270-98-0 1271-19-8 11079-20-2 11079-32-6

52700-41-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(partial retention of diat. differential overlap MO calcns. of, conformation in relation to)

L31 ANSWER 36 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1989:407542 Document No. 111:7542 (Cyclopentadienyl)zirconium hydride complexes with β -diketonate ligands. Strunkina, L. I.; Klemenkova, Z. M.; Lokshin, B. V.; Brainina, E. M. (Inst. Elementoorg. Soedin., Moscow, USSR). Metalloorganicheskaya Khimiya, 1(2), 389-91 (Russian) 1988. CODEN: MEKHEX. ISSN: 0235-0114.

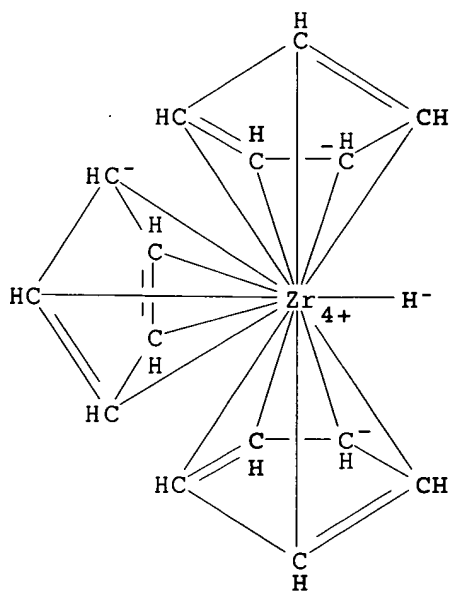
AB Disproportionation reaction of $(\text{RCOCHCOR1})_4\text{Zr}$ (I; R = R1 = Me, Ph; R = Me, R1 = Ph) with Cp_2ZrH_2 (Cp = cyclopentadienyl) gave 88-99% $\text{Cp}_2\text{Zr}(\text{RCOCHCOR1})_2\text{H}$. Treating I (R = R1 = Me, Ph) with Cp_2ZrD_2 gave $\text{Cp}_2\text{Zr}(\text{RCOCHCOR1})_2\text{D}$.

IT 78446-26-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 78446-26-1 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)hydro- (9CI) (CA INDEX NAME)

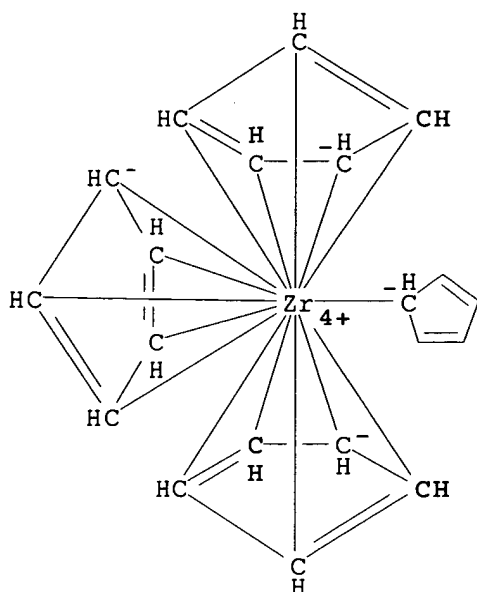


IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with zirconocene dihydride)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 12216-18-1P **78446-26-1P** 121116-42-5P 121116-43-6P

121116-44-7P 121131-01-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **1273-01-4**, Tetrakis(cyclopentadienyl)zirconium 17455-33-3

17500-78-6 17501-44-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with zirconocene dihydride)

L31 ANSWER 37 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1988:528708 Document No. 109:128708 Synthesis of cis-9-tricosene, a known sex pheromone. Byers, Jim D.; Drake, Charles A. (Phillips Petroleum Co., USA). U.S. US 4749818 A **19880607**, 4 pp. (English). CODEN: USXXAM. APPLICATION: US 1987-103764 19870930.

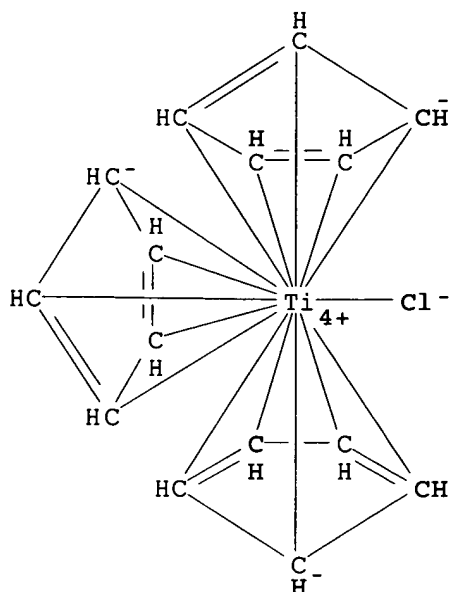
AB Title compd. (I), a known sex pheromone for the common housefly, is prepd. by metalating cis-H₂C:CH(CH₂)₆CH:CH(CH₂)₇Me [cis-(II)] with an organomagnesium halide to the cis-9-octadecenylmagnesium halide, followed by alkylation with n-pentyl halide. Oleyl alc. (4:1 cis-trans ratio) was dehydrated over γ alumina to give cis- and trans-II (4:1) which was treated with BuMgCl in presence of titanocene dichloride and alkylated with Me(CH₂)₃CH₂Br in the presence of CuBr to give I.

IT **11079-20-2**

RL: CAT (Catalyst use); USES (Uses)
(metalation catalysts, for octadecadiene)

RN 11079-20-2 HCAPLUS

CN Titanium, chlorotris(η⁵-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



IC ICM C07C001-00

INCL 585324000

CC 26-2 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 5

IT 1271-19-8, Titanocene dichloride 7550-45-0, Titanium tetrachloride, uses and miscellaneous 11079-20-2

RL: CAT (Catalyst use); USES (Uses)

(metalation catalysts, for octadecadiene)

L31 ANSWER 38 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1988:493213 Document No. 109:93213 Nitrate and hydroxyl derivatives of cyclopentadienyl zirconium complexes. Brainina, E. M.; Minacheva, M. Kh.; Klemenkova, Z. S.; Lokshin, B. V.; Mikhailova, O. A. (Inst. Elementoorg. Soedin., Moscow, USSR). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (8), 1848-51 (Russian) 1987. CODEN: IASKA6. ISSN: 0002-3353. OTHER SOURCES: CASREACT 109:93213.

AB Treating Cp₄Zr (Cp = cyclopentadienyl) with 54% HNO₃ gave 70%

Cp₂Zr(NO₃)(OH)·H₂O which on treatment with H₂O gave 58%

[Cp₂Zr(NO₃)(OH)₂·H₂O]₄ (I). Treating I with HNO₃ gave 40%

Cp₂Zr(NO₃)₂(OH), also prepd. in 60% yield from Cp₂Zr(NO₃)₂ and H₂O.

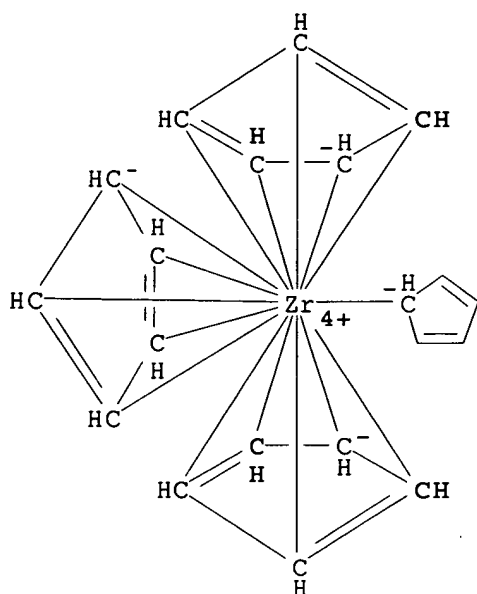
IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with nitric acid)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 1273-01-4, Tetrakis(cyclopentadienyl)zirconium

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nitric acid)

L31 ANSWER 39 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1988:406658 Document No. 109:6658 ESR study of the interaction between hydrides of cyclopentadienylzirconium complexes and spin traps.

Gasnov, R. G.; Strunkina, L. I.; Brainina, E. M. (Inst. Elementoorg. Soedin., Moscow, USSR). Doklady Akademii Nauk SSSR, 294(5), 1146-50 [Phys. Chem.] (Russian) 1987. CODEN: DANKAS. ISSN: 0002-3264.

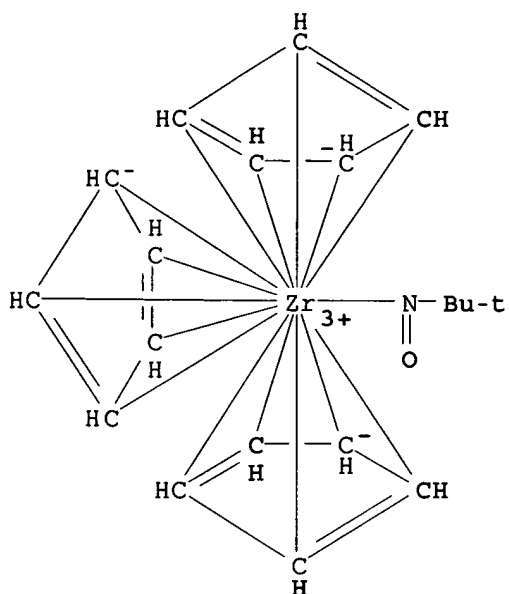
AB Reaction of Cp_2ZrH_2 ($\text{Cp} = \eta^5\text{-cyclopentadienyl}$), Cp_2ZrHCl , or Cp_3ZrH with spin traps (e.g., Me_3CNO , PhCH:NOCMe_3) in PhMe or C_6H_6 gave radicals $\text{RN}(\text{O})\bullet\text{R}_1$ [$\text{R} = \text{Cp}_2\text{ZrH}$, Cp_2ZrCl , Cp_3Zr , H , PhCH_2 , $\text{Cp}_2\text{Zr}(\text{PhHCl})$; $\text{R}_1 = \text{CMe}_3$, $\text{C}_6\text{H}_2(\text{CMe}_3)_3$ -2,4,6, C_6HMe_4 -2,3,5,6] for which ESR spectral data are reported.

IT 114663-88-6P

RL: PRP (Properties); PREP (Preparation)
(formation and ESR spectrum of)

RN 114663-88-6 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl) (2-methyl-2-nitrosopropane-N)-(9CI) (CA INDEX NAME)



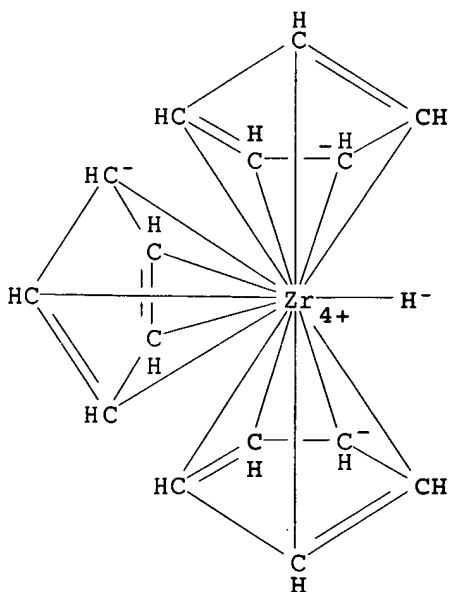
IT 78446-26-1, Tris(cyclopentadienyl)zirconium hydride

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with spin traps)

RN 78446-26-1 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)hydro- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 77

IT 24293-08-1P 40489-75-6P 74070-76-1P 83435-40-9P 103124-93-2P

114663-86-4P 114663-87-5P 114663-88-6P 114663-89-7P

RL: PRP (Properties); PREP (Preparation)

(formation and ESR spectrum of)

IT 37342-97-5, Zirconocene chloride hydride 37342-98-6
 78446-26-1, Tris(cyclopentadienyl)zirconium hydride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with spin traps)

L31 ANSWER 40 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1987:598963 Document No. 107:198963 Unusual possibilities of polymerization on "metallocene/aluminoxane" - type highly active catalysts. Kaminsky, W.; Miri, M. (Inst. Tech. Macromol., Hamburg, Fed. Rep. Ger.). Mezhdunar. Simp. Svyazi Gomogennym Geterog. Katal., 5th, Volume 2, Issue 1, 25-39. Editor(s): Ermakov, Yu. I.; Likholobov, V. A. Akad. Nauk SSSR, Sib. Otd., Inst. Katal.: Novosibirsk, USSR. (Russian) 1986. CODEN: 55TGA9.

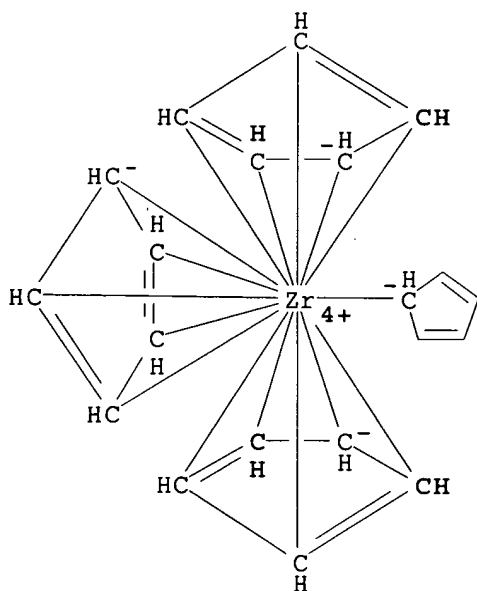
AB Zr and Ti metallocenes with methylaluminoxanes were sol. Ziegler catalysts with high activity and gave polyethylene with a no. of special properties. During polymn. of ethylene with hexene in the presence of such catalysts, chains with exclusively head-to-tail addn. were formed. During the polymn. of propylene, catalysts contg. Cp₂ZrCl₂ (Cp = cyclopentadienyl) gave only the atactic polymer.

IT 1273-01-4

RL: CAT (Catalyst use); USES (Uses)
 (catalysts, contg. aluminoxane, for polymn. of olefins)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

IT 1271-19-8 1271-66-5 1273-01-4 1291-32-3 1291-45-8
 12097-04-0 12636-72-5 37260-88-1 54039-38-2 79169-19-0
 109665-58-9

RL: CAT (Catalyst use); USES (Uses)
 (catalysts, contg. aluminoxane, for polymn. of olefins)

L31 ANSWER 41 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1987:5172 Document No. 106:5172 ESR study of the reaction of zirconium cyclopentadienyl hydride complexes with benzyl halides in the presence of 2,4,6-tri-tert-butyl nitrosobenzene. Freidlina, R. Kh.; Gasanov, R. G.; Strunkina, L. I.; Brainina, E. M. (Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (6), 1452-3 (Russian) 1986. CODEN: IASKA6. ISSN: 0002-3353.

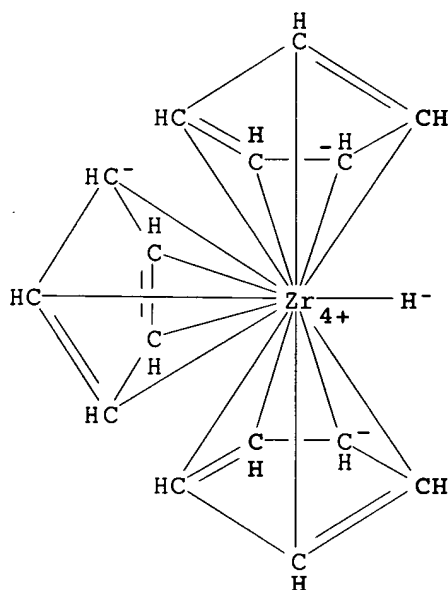
AB A spin-trapping study showed that π -cyclopentadienylzirconium hydrides react with PhCH_2X (I; X = Cl, Br) by abstraction of X^\bullet from I.

IT 78446-26-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzyl halides, spin-trapping study of)

RN 78446-26-1 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)hydro- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

IT 37342-97-5 37342-98-6 78446-26-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzyl halides, spin-trapping study of)

L31 ANSWER 42 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

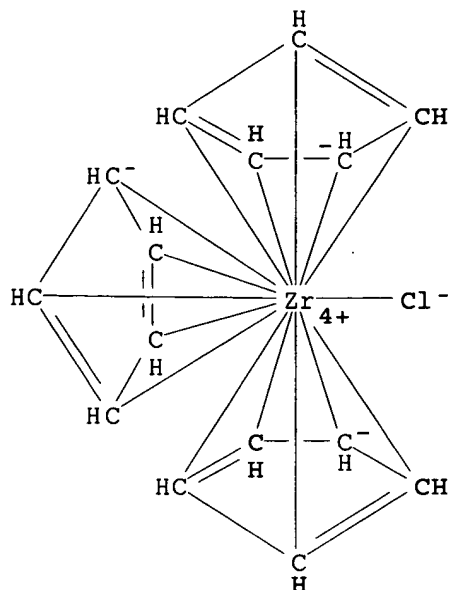
1986:553243 Document No. 105:153243 Part I. New ferrocenyl thio and seleno ether ligands. Preparation, characterization, and their palladium(II) complexes as catalysts for selective hydrogenation and Grignard cross-coupling. Part II. The synthesis of tris(cyclopentadienyl)zirconium chloride and the photolyses of $\text{Cp}_2\text{TiIII}(\text{CO})_2$ and $(\text{Cp}_2\text{ZrIVCl})_2\text{O}$. Shen, Lie Hang (Michigan State Univ., East Lansing, MI, USA). 424 pp. Avail. Univ. Microfilms Int., Order No. DA8603479 From: Diss. Abstr. Int. B 1986, 46(12), Pt. 1, 4238 (English) 1985.

AB Unavailable

IT 62343-37-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)
 RN 62343-37-7 HCAPLUS
 CN Zirconium, chlorotris(η^5 -2,4-cyclopentadien-1-yl)- (9CI) (CA
 INDEX NAME)



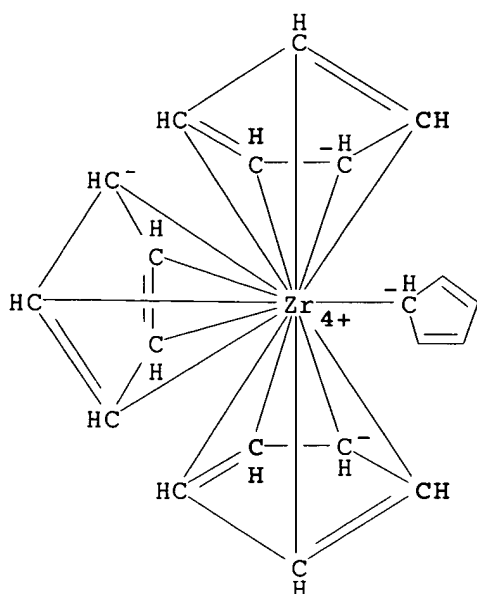
CC 29-12 (Organometallic and Organometalloidal Compounds)
 IT 62343-37-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

L31 ANSWER 43 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
 1986:553177 Document No. 105:153177 Chemistry of transition metal
 alkyl compounds. XLIII. Reduction of organozirconium(IV) compounds
 with organolithium reagents. Thiele, K. H.; Krueger, A. (Sekt.
 Chem., Tech. Hochsch. "Carl Schorlemmer", Merseburg, DDR-4200, Ger.
 Dem. Rep.). Zeitschrift fuer Anorganische und Allgemeine Chemie,
 527, 95-8 (German) 1985. CODEN: ZAACAB. ISSN: 0044-2313.
 OTHER SOURCES: CASREACT 105:153177.

AB The 1:1 reaction of $(C_5H_5)_2ZrPh_2$ (I) with $PhLi$ (II) in Et_2O gave
 $C_5H_5ZrPh_2 \cdot 2.0Et_2$. Similarly, $(C_5H_5)_2Zr(CH_2Ph)_2$ and $PhCH_2Li$ gave 35%
 $C_5H_5Zr(CH_2Ph)_2 \cdot 2.0Et_2$. The 1:2 reaction of I-II gave 45%
 $C_5H_5ZrPh_3 \cdot 3.0Et_2$.

IT 1273-01-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (redn. of, with phenyllithium)

RN 1273-01-4 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-
 yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(redn. of, with phenyllithium)

L31 ANSWER 44 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1985:523628 Document No. 103:123628 The preparation and catalytic applications of supported zirconocene and hafnocene complexes. Chang, Biau Hung; Grubbs, Robert H.; Brubaker, Carl H., Jr. (Dep. Chem., Michigan State Univ., East Lansing, MI, 48824, USA). Journal of Organometallic Chemistry, 280(3), 365-76 (English) 1985 . CODEN: JORCAI. ISSN: 0022-328X. OTHER SOURCES: CASREACT 103:123628.

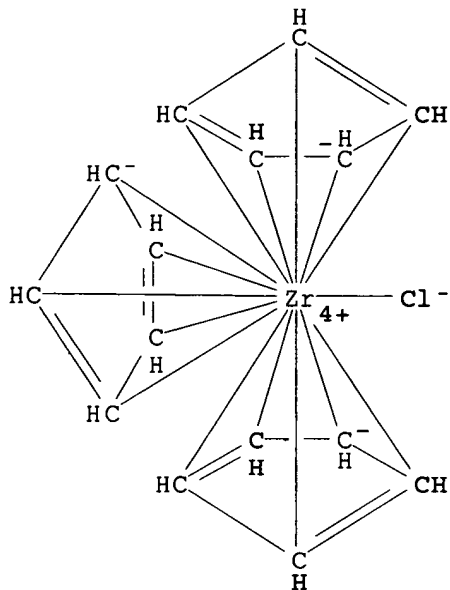
AB Polymer-attached Cp₂ZrCl₂, Cp₂HfCl₂, CpZrCl₃, CpHfCl₃, Cp₃ZrCl and Cp₃HfCl (Cp = cyclopentadienyl) have been prepd. The polymer-attached Cp₂ZrCl₂, on redn. with BuLi, produced an active catalyst whose efficiency for olefin hydrogenation is about eight times as great as that of the corresponding homogeneous species under the same conditions. The redn. products of supported zirconocene and hafnocene complexes are active hydrogenation catalysts for diphenylacetylene which was hydrogenated to 1,2-diphenylethane through intermediate stilbene. The similar redn. products have also been employed in catalytic isomerization of allylbenzene, cis-stilbene and 1,5-cyclooctadiene. Allylbenzene was converted into a mixt. of trans- and cis-propenylbenzene, cis-stilbene was isomerized to trans-stilbene, and 1,5-cyclooctadiene was isomerized to 1,3-cyclooctadiene through the 1,4-cyclooctadiene intermediate. Polymer-attached Cp₂ZrCl₂, CpZrCl₃, Cp₂HfCl₂, and CpHfCl₃ can be used directly, without going through the redn. process, for the low yield epoxidn. of cyclohexene. Polymer-attached Cp₂ZrCl₂ was used in hydrozirconation and carbon monoxide redn. studies.

IT 62343-37-7DP, polymer supported 97365-62-3DP, polymer supported

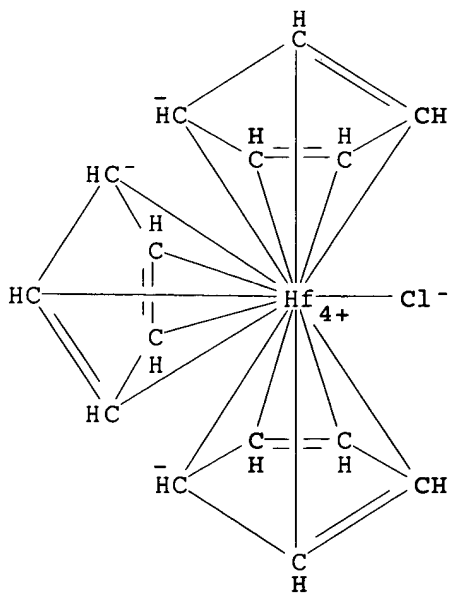
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. and catalytic activity of)

RN 62343-37-7 HCAPLUS
 CN Zirconium, chlorotris(η^5 -2,4-cyclopentadien-1-yl) - (9CI) (CA
 INDEX NAME)



RN 97365-62-3 HCAPLUS
 CN Hafnium, chlorotris(η^5 -2,4-cyclopentadien-1-yl) - (9CI) (CA
 INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 25, 67
 IT 1291-32-3DP, polymer supported 12116-66-4DP, polymer supported

34767-44-7DP, polymer supported 61906-04-5DP, polymer supported
62343-37-7DP, polymer supported 97365-62-3DP,
polymer supported

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
(prepn. and catalytic activity of)

L31 ANSWER 45 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1985:166292 Document No. 102:166292 Reduction of trichloromethyl
groups in polychloroalkanes by hydride complexes of
cyclopentadienylzirconium. Brainina, E. M.; Strunkina, L. I.;
Kuz'mina, N. A.; Grechkina, E. M. (Inst. Elementoorg. Soedin.,
Moscow, USSR). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya
(1), 228-31 (Russian) 1985. CODEN: IASKA6. ISSN:
0002-3353. OTHER SOURCES: CASREACT 102:166292.

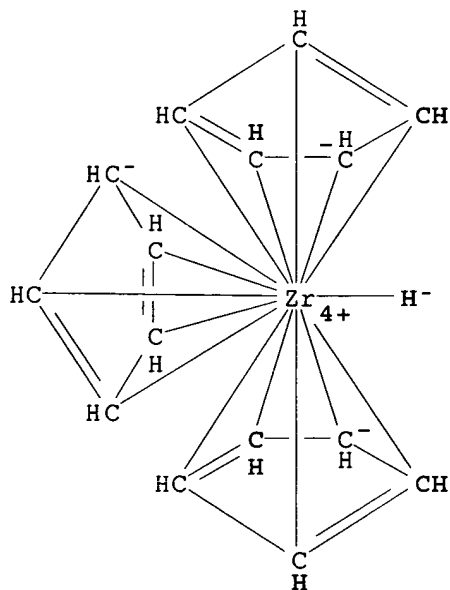
AB Cp₃ZrH (Cp = cyclopentadienyl), Cp₂ZrH₂, and CpZrClH reduced the
Cl₃C group in Cl₃C(CH₂)₆Me, Cl₃CCH₂CH₂Cl, and Cl₃CCHCl₂ to give the
corresponding Cl₂CH compds.

IT 78446-26-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive dechlorination by, of trichloromethyl group in
polychloroalkanes)

RN 78446-26-1 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)hydro- (9CI) (CA
INDEX NAME)



CC 23-3 (Aliphatic Compounds)

IT 37342-97-5 37342-98-6 78446-26-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive dechlorination by, of trichloromethyl group in
polychloroalkanes)

L31 ANSWER 46 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1985:78926 Document No. 102:78926 Steric factor dependence of the
structures of certain Cp-containing compounds. Lobkovskii, E. B.
(Inst. New Chem. Probl., Chernogolovka, 142432, USSR). Journal of

Organometallic Chemistry, 277(1), 53-9 (English) 1984.

CODEN: JORCAI. ISSN: 0022-328X.

- AB The structures of the title compds. MCpn (M = Be, Fe, Cr, V, Li, Sc, Nd, etc.; Cp = cyclopentadienyl; n = 2, 3, 4) were discussed in terms of steric hindrance. If the sum of normalized solid angles $\Sigma(S_i/r_i^2)$ ($i = 1-n$ and r_i = radius of ligand, S_i = area of ligand) exceeds unity or is appreciably less unity, structural rearrangement occur in the mol. E.g., if in the mol. BeCp₂, both Cp rings are bonded with the Be through π -bonds, then the sum of the angles = 1.09. This steric hindrance is removed by shifting of the rings and in the actual mol., the sum of angles = 0.92.

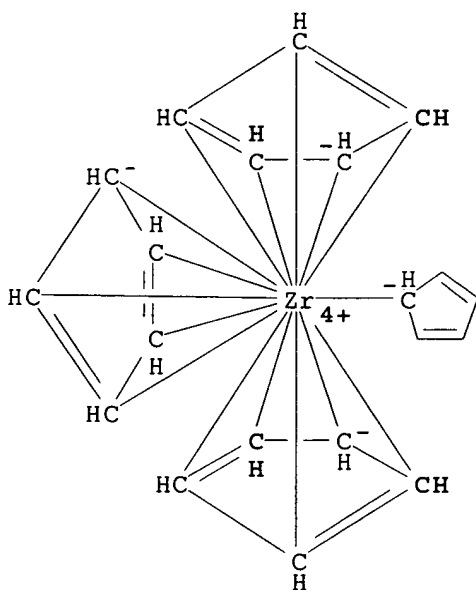
IT 1273-01-4

RL: PRP (Properties)

(mol. structure of, steric hindrance in relation to)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-1 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

IT 102-54-5 1271-24-5 1271-29-0 1273-01-4 1273-98-9
 1277-47-0 1293-75-0 1298-54-0 1298-55-1 1298-76-6
 12149-28-9 12701-79-0 29941-03-5 37048-03-6 52550-20-6
 52700-41-1 63726-15-8

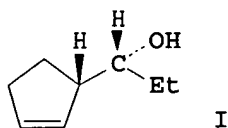
RL: PRP (Properties)

(mol. structure of, steric hindrance in relation to)

L31 ANSWER 47 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1984:591195 Document No. 101:191195 Regio- and stereoselective reaction of 1,3-dialkyl-substituted allyl anions with aldehydes via η^3 -allyltitanium compounds. Kobayashi, Yuichi; Umeyama, Kensuke; Sato, Fumie (Dep. Chem. Eng., Tokyo Inst. Technol., Tokyo, 152, Japan). Journal of the Chemical Society, Chemical Communications (9), 621-3 (English) 1984. CODEN: JCCCAT. ISSN: 0022-4936. OTHER SOURCES: CASREACT 101:191195.

GI



AB The regio- and stereochem. in reactions of 1,3-dialkyl-substituted allyl anions with aldehydes is controlled via η^3 -allyltitanium compds., thus providing a simple method for the prepn. of cycloalkanes having 1-hydroxyalkyl side chains. Thus, $(\eta^5\text{-Cp})_2\text{TiCl}$ (Cp = cyclopentadienyl), formed in situ by reaction of $(\eta^5\text{-Cp})_2\text{TiCl}_2$ with $\text{Me}_2\text{CHCH}_2\text{MgCl}$ in THF at room temp., reacted with $\text{Me}_2\text{CHCH}_2\text{MgCl}$ in the presence of cyclopentadiene in THF at -40° for 10 min to give the corresponding allyltitanium compd., which was treated with EtCHO to give 86% of the erythro isomer I exclusively.

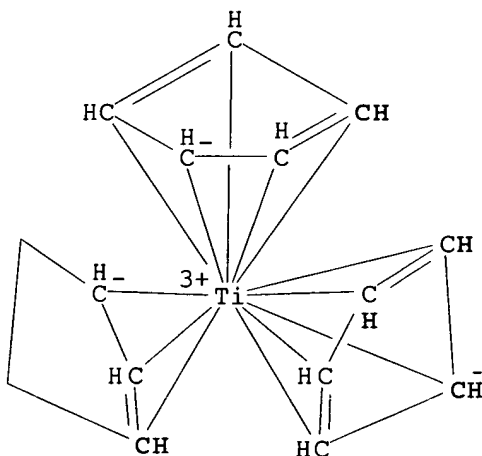
IT 92362-14-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, with propionaldehyde, stereoselectivity of)

RN 92362-14-6 HCAPLUS

CN Titanium, bis(η^5 -2,4-cyclopentadien-1-yl) [(1,2,3- η)-2-cyclopenten-1-yl]- (9CI) (CA INDEX NAME)



CC 24-6 (Alicyclic Compounds)

Section cross-reference(s): 22, 23, 29

IT 92362-08-8P 92362-09-9P 92362-10-2P 92362-11-3P 92362-12-4P
92362-13-5P 92362-14-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, with propionaldehyde, stereoselectivity of)

L31 ANSWER 48 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1984:34089 Document No. 100:34089 Reduction of carbon tetrachloride and trichloromethane by cyclopentadienyl complexes of zirconium and

hafnium hydrides. Strunkina, L. I.; Brainina, E. M. (Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (9), 2160-2 (Russian) 1983. CODEN: IASKA6. ISSN: 0002-3353.

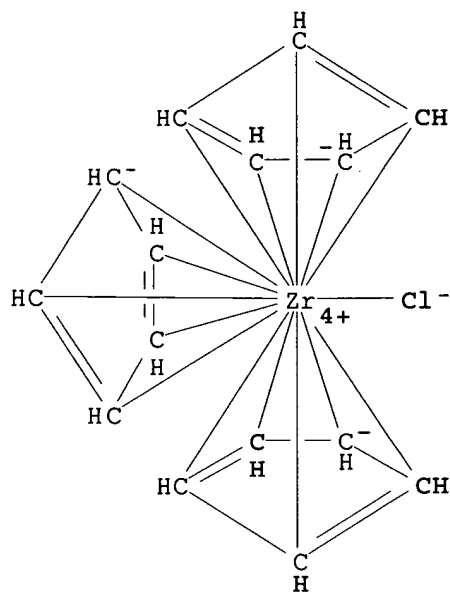
AB Cp_3MH ($\text{Cp} = \eta^5\text{-cyclopentadienyl}$; $\text{M} = \text{Zr}, \text{Hf}$) and Cp_2ZrClH reduced CCl_4 and CHCl_3 in PhMe to CHCl_3 and CH_2Cl_2 , resp.

IT 62343-37-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, in redn. of carbon tetrachloride by cyclopentadienylzirconium hydride)

RN 62343-37-7 HCAPLUS

CN Zirconium, chlorotris($\eta^5\text{-2,4-cyclopentadien-1-yl}$)- (9CI) (CA INDEX NAME)

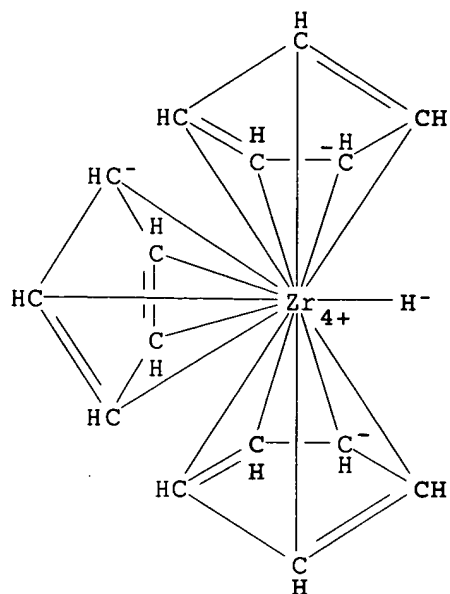


IT 78446-26-1 84101-40-6

RL: RCT (Reactant); RACT (Reactant or reagent) (redn. of carbon tetrachloride and chloroform with)

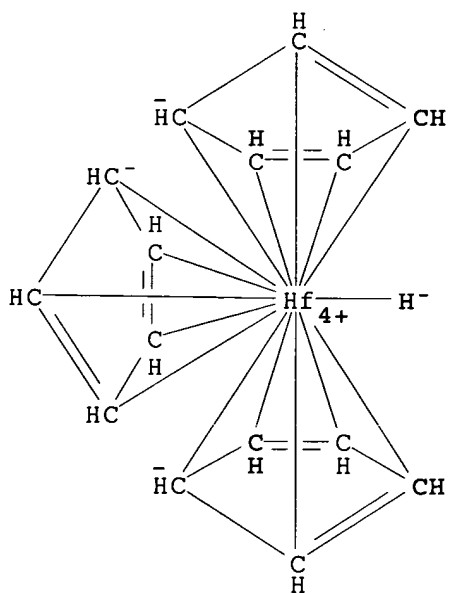
RN 78446-26-1 HCAPLUS

CN Zirconium, tris($\eta^5\text{-2,4-cyclopentadien-1-yl}$)hydro- (9CI) (CA INDEX NAME)



RN 84101-40-6 HCAPLUS

CN Hafnium, tris(η5-2,4-cyclopentadien-1-yl)hydro- (9CI) (CA INDEX NAME)



CC 23-3 (Aliphatic Compounds)
Section cross-reference(s): 29

IT 62343-37-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, in redn. of carbon tetrachloride by
cyclopentadienylzirconium hydride)

IT 37342-97-5 78446-26-1 84101-40-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(redn. of carbon tetrachloride and chloroform with)

L31 ANSWER 49 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1983:34673 Document No. 98:34673 Vibrational spectra of tris(cyclopentadienyl)zirconium and -hafnium hydrides and deuterides, Cp₃MX (M = Zr, Hf; X = H, D). Lokshin, B. V.; Klemenkova, Z. S.; Ezernitskaya, M. G.; Strunkina, L. I.; Brainina, E. M. (A. N. Nesmeyanov Inst. Organoelem. Compd., Moscow, 117813, USSR). Journal of Organometallic Chemistry, 235(1), 69-75 (English) 1982. CODEN: JORCAI. ISSN: 0022-328X.

AB Cp₃HfX (X = H, D; Cp = η^5 cyclopentadienyl) were prepd. by treating Cp₄Hf with LiAlX₄. The IR and Raman spectra of Cp₃MX (I, M = Zr, Hf; X = H, D) were studied. I have 3 identically bonded cyclopentadienyl ligands. The spectral characteristics are consistent with metal-ring coordination. An increase is noted in the strength of the M-CH and M-Cp bonds when passing from Zr to Hf.

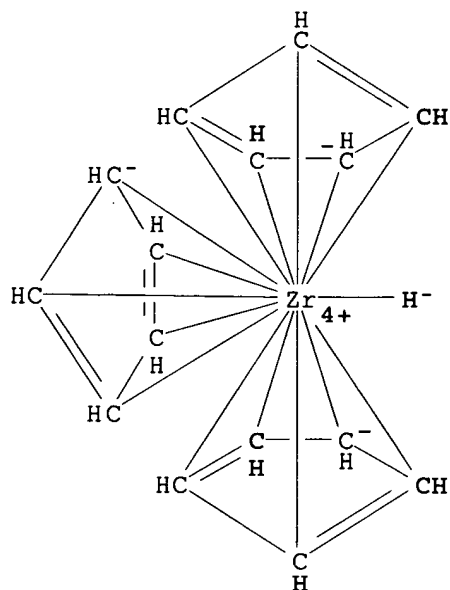
IT 78446-26-1 78446-27-2

RL: PRP (Properties)

(IR and Raman spectra of)

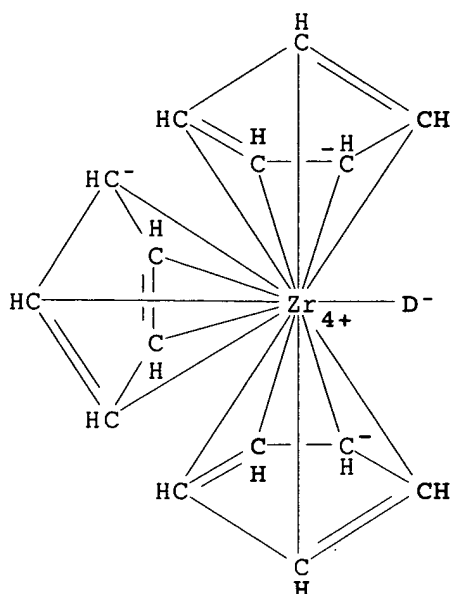
RN 78446-26-1 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)hydro- (9CI) (CA INDEX NAME)



RN 78446-27-2 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)hydro-d- (9CI) (CA INDEX NAME)

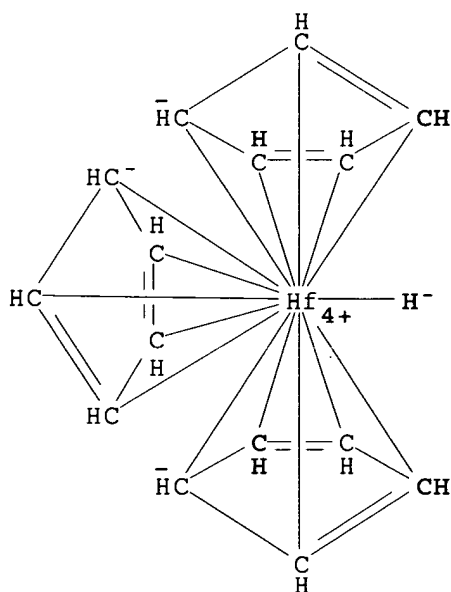


IT 84101-40-6P 84101-41-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and IR and Raman spectra of)

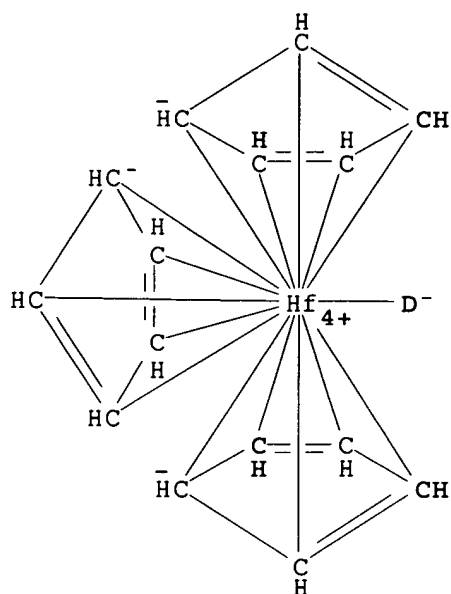
RN 84101-40-6 HCAPLUS

CN Hafnium, tris(η5-2,4-cyclopentadien-1-yl)hydro- (9CI) (CA INDEX
NAME)



RN 84101-41-7 HCAPLUS

CN Hafnium, tris(η5-2,4-cyclopentadien-1-yl)hydro-d- (9CI) (CA
INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 78446-26-1 78446-27-2

RL: PRP (Properties)

(IR and Raman spectra of)

IT 84101-40-6P 84101-41-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and IR and Raman spectra of)

L31 ANSWER 50 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1981:551475 Document No. 95:151475 Starch-polyolefin polymer compositions. Kaminsky, Walter (Maizena G.m.b.H., Fed. Rep. Ger.). Ger. Offen. DE 3007433 19810903, 12 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1980-3007433 19800228.

AB Low-mol. wt. aliph. α -monoolefins are polymd. in an inert liq. and(or) gaseous reaction medium at -50 to 140° using halogen-free Ziegler-Natta catalysts prepd. by treating starch (I) with a trialkylaluminum and a transition metal compd. The catalysts are less corrosive than conventional catalysts and smaller amts. are needed to achieve the same activity and productivity achieved with larger amts. of conventional catalysts. Thus, 19.6 g starch in 250 mL toluene was treated with 200 mmol Me₃Al [75-24-1] at 40°. After 40 min, 0.05 mmol bis(cyclopentadienyl)dimethyltitanium [1271-66-5] was added and ethylene was admitted to a pressure of 9 bar. Polymn. for 1 h gave 49.6 g I-polymer compn. contg. 19.6 g I and 30 g polyethylene (II) [9002-88-4]. The catalyst productivity was 14,300 g II/g Ti, vs. 30-60 g II/g Ti for a conventional catalyst. The I-II compn. could be used for the prodn. of industrial materials with better properties than could be achieved with mech. blends of I and II, or the starch could be dissolved out by conventional methods.

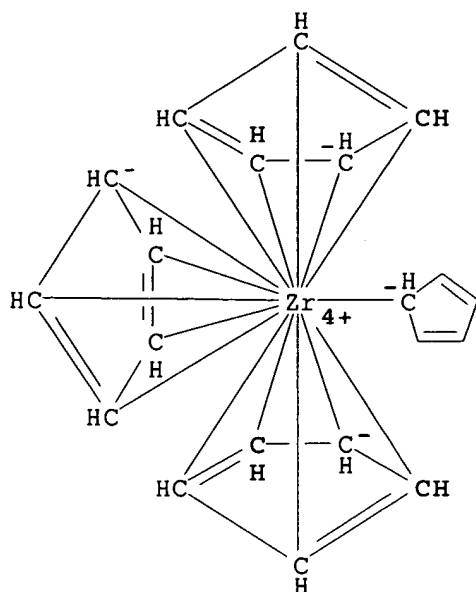
IT 1273-01-4

RL: CAT (Catalyst use); USES (Uses)

(catalysts, contg. alkyl aluminum compds. and starch, for polymn. of olefins)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η 5-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



IC C08F010-00

CC 35-4 (Synthetic High Polymers)

IT 1273-01-4

RL: CAT (Catalyst use); USES (Uses)

(catalysts, contg. alkyl aluminum compds. and starch, for polymn. of olefins)

L31 ANSWER 51 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1981:462334 Document No. 95:62334 Tris(cyclopentadienyl)zirconium hydride ($\eta^5\text{-C}_5\text{H}_5$) $_3\text{ZrH}$. Brainina, E. M.; Strunkina, L. I.; Lokshin, B. V.; Ezernitskaya, M. G. (Inst. Elementoorg. Soedin. im. Nesmeyanova, Moscow, USSR). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (2), 447-9 (Russian) 1981. CODEN: IASKA6. ISSN: 0002-3353.

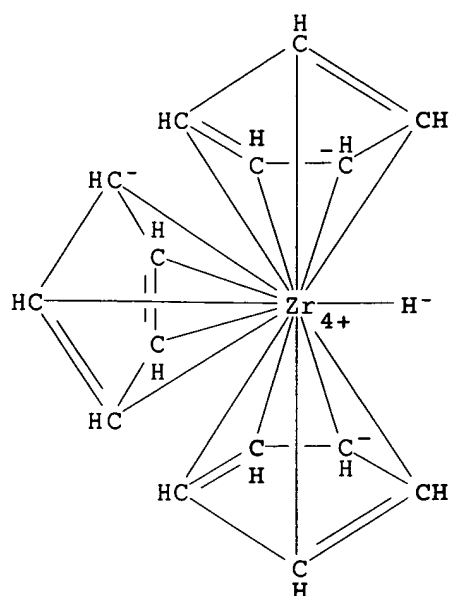
AB ($\eta^5\text{-C}_5\text{H}_5$) $_3\text{ZrR}$ (R = H, D) were prepd. in 42, 11% yields resp. by treating ($\eta^5\text{-C}_5\text{H}_5$) $_4\text{Zr}$ with LiAlR_4 in THF at 20°.

IT 78446-26-1P 78446-27-2P

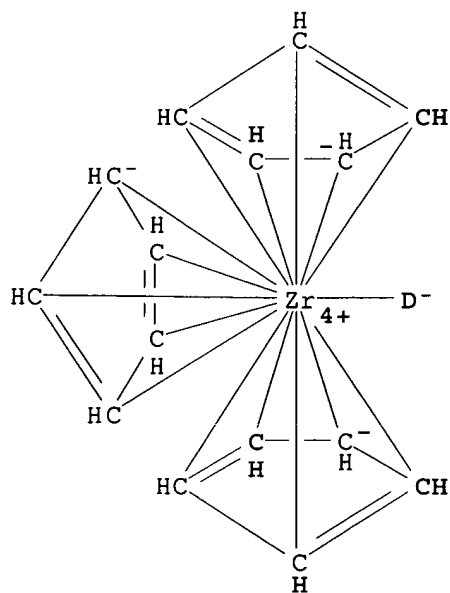
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 78446-26-1 HCAPLUS

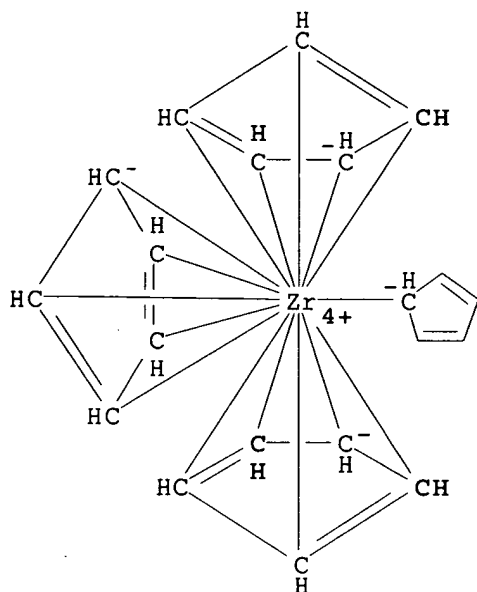
CN Zirconium, tris($\eta^5\text{-2,4-cyclopentadien-1-yl}$)hydro- (9CI) (CA INDEX NAME)



RN 78446-27-2 HCAPLUS
 CN Zirconium, tris(η5-2,4-cyclopentadien-1-yl)hydro-d- (9CI) (CA INDEX NAME)



IT 1273-01-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (redn. of)
 RN 1273-01-4 HCAPLUS
 CN Zirconium, tris(η5-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 78446-26-1P 78446-27-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(redn. of)

L31 ANSWER 52 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1981:182985 Document No. 94:182985 Zirconium-91 nuclear magnetic resonance spectroscopy: the first chemical study. Sayer, Brian G.; Hao, Nguyen; Denes, Georges; Bickley, Douglas G.; McGlinchey, Michael J. (Dep. Chem., McMaster Univ., Hamilton, ON, L8S 4M1, Can.). Inorganica Chimica Acta, 48(1), 53-5 (English) 1981
. CODEN: ICHAA3. ISSN: 0020-1693.

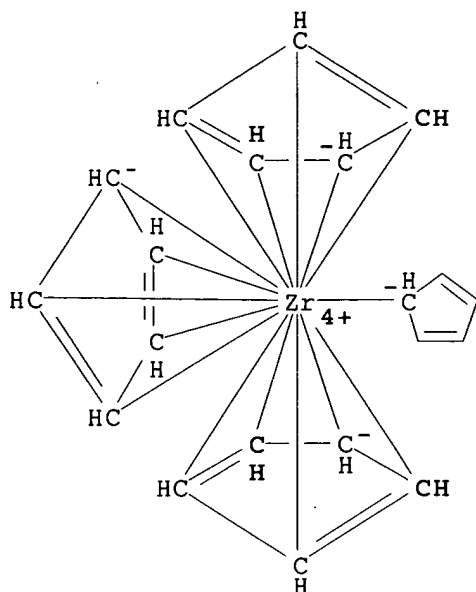
AB 91Zr NMR signals were obsd. for the series Cp₂ZrX₂ (Cp = cyclopentadienyl; X = Cl, Br, I) and ZrX₆²⁻ (X = F, Cl) ions, and an inverse halogen dependence was found. The ¹³C NMR of the fluxional mol. Cp₄Zr is also reported.

IT 1273-01-4

RL: PRP (Properties)
(NMR of zirconium-91 in)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 73-4 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)

IT 1273-01-4 1291-32-3 1294-67-3 1298-41-5 16919-31-6
44493-89-2 60897-78-1

RL: PRP (Properties)
(NMR of zirconium-91 in)

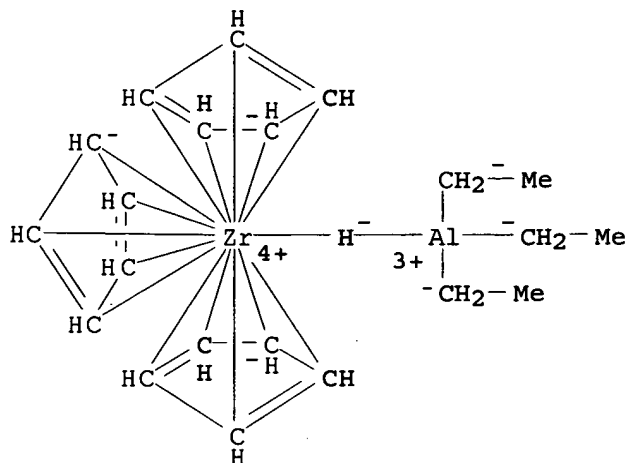
L31 ANSWER 53 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1981:39825 Document No. 94:39825 Al,Zr- μ -hydrido(triethylaluminum) [tri(cyclopentadienyl)zirconium(IV)], C₂₁H₃₁AlZr. Kopf, J.; Vollmer, H. J.; Kaminsky, W. (Inst. Anorg. Angew. Chem., Univ. Hamburg, Hamburg, D-2000/13, Fed. Rep. Ger.). Crystal Structure Communications, 9(4), 985-90 (English)
1980. CODEN: CSCMCS. ISSN: 0302-1742.

AB The title compd. is orthorhombic, space group Pcmn, with a 804.2(2), b 1328.6(6), and c 1904.7(7) pm; d. (calcd.) = 1.31 for Z = 4. Final R = 0.077 (Rw = 0.083). A striping feature of the mol. structure is the relatively short C-C bond length of 144.3 pm and the increased C-C-Al angle of 134° of one Et group.

IT 73505-54-1
RL: PRP (Properties)
(crystal structure of)

RN 73505-54-1 HCAPLUS
CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)- μ -hydro(triethylaluminum) - (9CI) (CA INDEX NAME)



CC 75-5 (Crystallization and Crystal Structure)

Section cross-reference(s): 29

IT 73505-54-1

RL: PRP (Properties)

(crystal structure of)

L31 ANSWER 54 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1980:472366 Document No. 93:72366 "Living polymers" with Ziegler catalysts of high productivity. Sinn, Hansjoerg; Kaminsky, Walter; Vollmer, Hans Juergen; Woldt, Ruediger (Inst. Anorg. Angewandte Chem., Univ. Hamburg, Hamburg, D-2000/13, Fed. Rep. Ger.). Angewandte Chemie, 92(5), 396-402 (German) 1980. CODEN: ANCEAD. ISSN: 0044-8249.

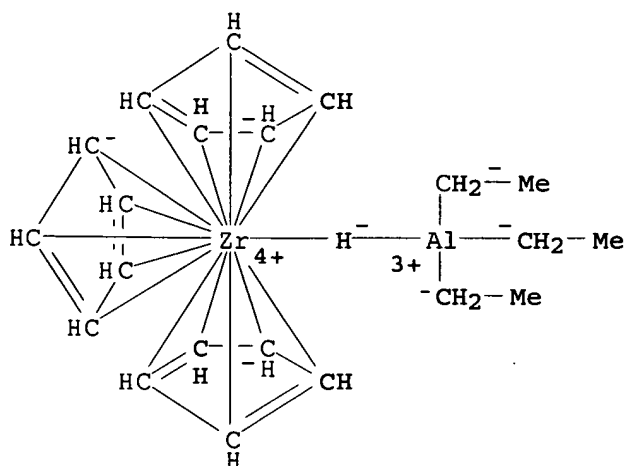
AB Polyethylene [9002-88-4] was obtained with high productivity, e.g. 107-108 g/g transition metal, in a living polymn.-type process in the presence of bis(cyclopentadienyl)dimethyltitanium(IV) [1271-66-5] or bis(cyclopentadienyl)dimethylzirconium(IV) (I) [12636-72-5] and methylaluminoxane. In the presence of I, the polymn. rate was linearly related to I concn. and a quadratic function of aluminoxane concn.

IT 73505-54-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 73505-54-1 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-μ-hydro(triethylaluminum) - (9CI) (CA INDEX NAME)

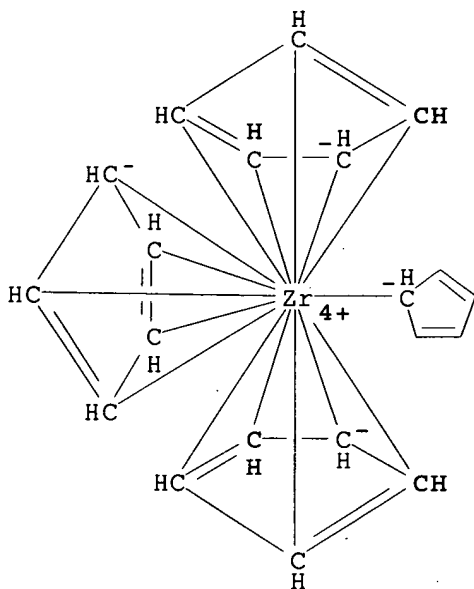


IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with triethylaluminum)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η5-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 35-4 (Synthetic High Polymers)

IT 73505-54-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with triethylaluminum)

L31 ANSWER 55 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1978:521350 Document No. 89:121350 Crystal and molecular structure of tetra(cyclopentadienyl)zirconium. Rogers, Robin D.; Bynum, R. Vann; Atwood, Jerry L. (Dep. Chem., Univ. Alabama, University, AL, USA). Journal of the American Chemical Society, 100(16), 5238-9 (English) 1978. CODEN: JACSAT. ISSN: 0002-7863.

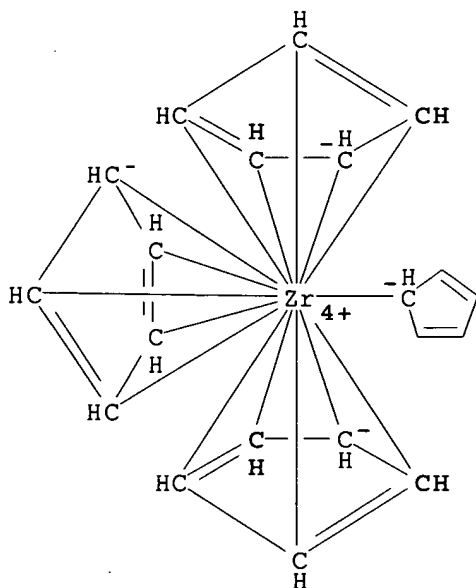
AB The long-standing controversy concerning the solid state structure of $(C_5H_5)_4Zr$ was resolved by a single-crystal x-ray diffraction study. There are 3 η^5 - C_5H_5 rings and 1 η^1 - C_5H_5 ligand. The compd. was reported by V. I. Kulishov et al. (1970) to be orthorhombic, space group $P2_12_12_1$. However, in this study it is monoclinic, space group $C2/c$, which indicates that the 2 compds are either of different cryst. modifications, one a twinned crystal, or different compds. The lattice consts. are a 13.332(5), b 9.065(4), c 25.684(6) Å, and β 103.40(3)°; d . (calcd.) = 1.53 for $Z = 8$. The structure was refined to a final $R = 0.046$ for 1461 reflections. The Zr-C(η^5) lengths av. 2.58(3) Å and are substantially longer than normal. The Zr-C(η^1) distance is 2.447(6) Å. For the sigma-bonded ring the Zr-C bond vector makes an angle of 49° with the plane of the C_5H_5 unit.

IT 1273-01-4

RL: PRP (Properties)
(structure of)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 75-5 (Crystallization and Crystal Structure)

Section cross-reference(s): 29

IT 1273-01-4

RL: PRP (Properties)
(structure of)

L31 ANSWER 56 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1977:552744 Document No. 87:152744 Polyethylene. Sinn, Hansjoerg; Mottweiler, Renke; Andresen, Arne; Cordes, Hans Guenther; Herwig, Jens; Kaminsky, Walter; Merck, Alexander; Vollmer, Hans Juergen;

Pein, Joachim (BASF A.-G., Fed. Rep. Ger.). Ger. Offen. DE 2608933 19770908, 10 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1976-2608933 19760304.

AB Ziegler catalysts are prepd. from cyclopentadienyl Zr compds. and Et₃Al [97-93-8] (1:0.001-20 mole ratio) for the manuf. of polyethylene (I) [9002-88-4] at -80 to +120°. The catalysts are halogen-free and, optionally, may contain H₂O for mol. wt. regulation. Thus, 0.1 mol tetrakis(cyclopentadienyl)zirconium [1273-01-4] was mixed with 0.7 mol Et₃Al at 60° until ethane evolution ceased (.apprx.1 wk) to give a dark red oil which was dild. to 300 mL with heptane. The catalyst (0.0022 mol/L Zr) was added to a reactor contg. 300 mL C₆H₆, the mixt. heated to 50°, and ethylene (9 bar) fed in. After 64 h, I yield was 81 g/L and the mol. wt. was 1,500,000.

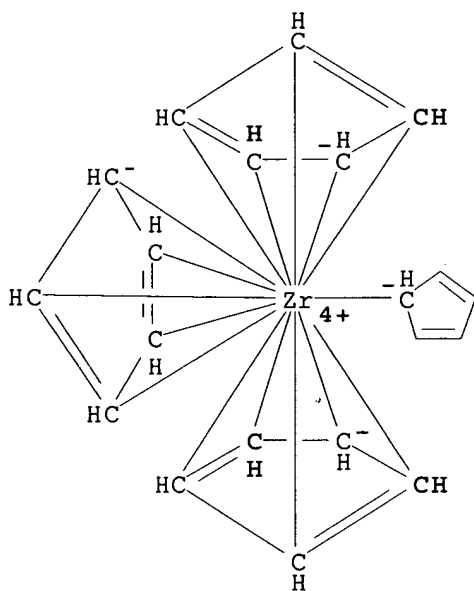
IT 1273-01-4 64539-44-2

RL: CAT (Catalyst use); USES (Uses)

(catalysts, contg. triethylaluminum, for ethylene polymn.)

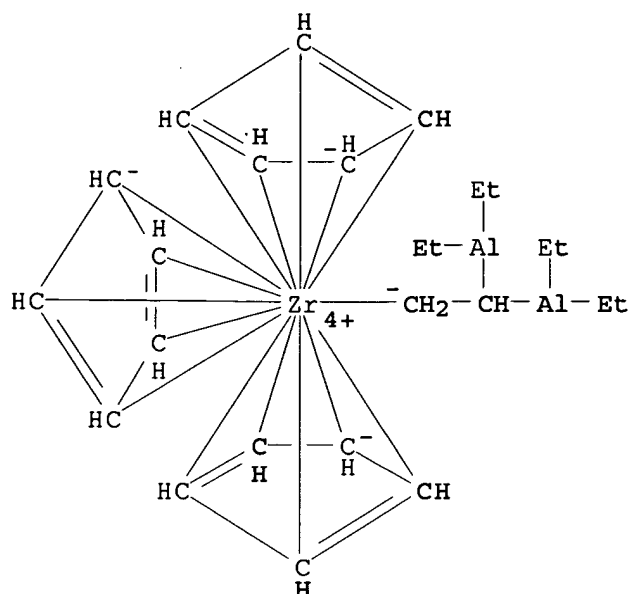
RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



RN 64539-44-2 HCAPLUS

CN Zirconium, [2,2-bis(diethylalumino)ethyl]tris(η⁵-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



IC C08F110-02

CC 35-4 (Synthetic High Polymers)

IT 1273-01-4 64539-44-2

RL: CAT (Catalyst use); USES (Uses)

(catalysts, contg. triethylaluminum, for ethylene polymn.)

L31 ANSWER 57 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1977:89965 Document No. 86:89965 Some aspects of zirconocene hydrochloride reactivity. Etievant, Patrick; Tainturier, Garard; Gautheron, Bernard (Lab. Organometall. Polarogr. Org., Fac. Sci. "Gabriel", Dijon, Fr.). Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques, 283(5), 233-6 (French) 1976. CODEN: CHDCAQ. ISSN: 0567-6541.

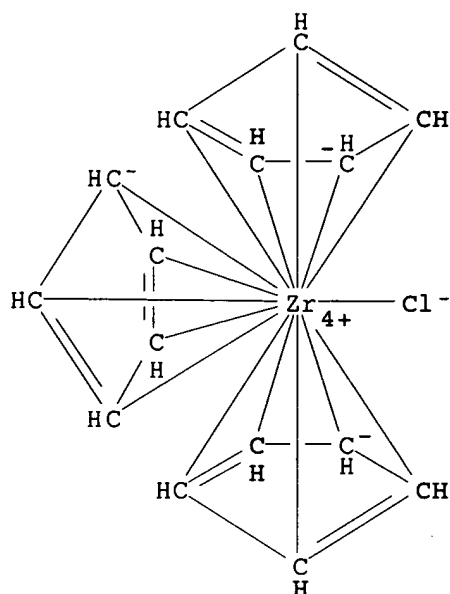
AB The title compds. formed complexes with ferrocene derivs., oxirane, CO₂, MeCN, PhCN, Ph₂CHCN, 2-MeC₆H₄OH, and cyclopentadiene. Some complexes of carbonyl compds. were hydrolyzed to the corresponding alcs. The complex with FcCOCH:CHMe (Fc = ferrocenyl) was hydrolyzed to 96% FcCH:CHCHMeOH and 4% FcCOPr.

IT 62343-37-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 62343-37-7 HCAPLUS

CN Zirconium, chlorotris(η⁵-2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 1271-94-9P 11087-28-8P 12097-04-0P 42378-22-3P 61993-59-7P

61993-60-0P 61993-61-1P 61993-62-2P 62053-83-2P

62343-37-7P 62343-40-2P 62343-41-3P 62343-42-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

L31 ANSWER 58 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1975:488167 Document No. 83:88167 Carbon-13 NMR spectra and structure of several chelate cyclopentadienyl compounds of zirconium and hafnium. Minacheva, M. Kh.; Arshavskaya, E. V.; Fedorov, L. A.; Brainina, E. M. (Inst. Elementoorg. Soedin., Moscow, USSR).

Koordinatsionnaya Khimiya, 1(6), 831-5 (Russian) 1975.

CODEN: KOKHDC. ISSN: 0132-344X.

AB The following complexes of Hf and Zr are studied by ^{13}C NMR spectra (213-300°K) to study their mol. structure: $\text{Cp}_4\text{Zr(I)}$, $\text{Cp}_2\text{ZrCl}_2\text{(IIa)}$, $\text{Cp}_2\text{HfCl}_2\text{(IIb)}$, $\text{CpZr(acac)}_2\text{Cl(IIIa)}$, $\text{CpZr(dbm)}_2\text{Cl(IIIb)}$, $\text{CpHf(dbm)}_2\text{(PhO)(IIIc)}$, $\text{CpZr(dbm)}_3\text{(IV)}$, and $\text{CpZr(acac)}_2\text{(dbm)(V)}$, where $\text{Cp} = \text{C}_5\text{H}_5$, $\text{acac} = \text{acetylacetonate}$, $\text{dbm} = \text{dibenzoylmethane}$. I is fluxional, those of type III are of a stereorigid cis-Cp-Cl pseudooctahedral structure. IV and V are pentagonal bipyramids with Cp in apical position. Two chelates in IV are in an equatorial position and they are equiv., and one chelate is bonded to one apical and one basal positions. V is probably a mixt. of conformational isomers.

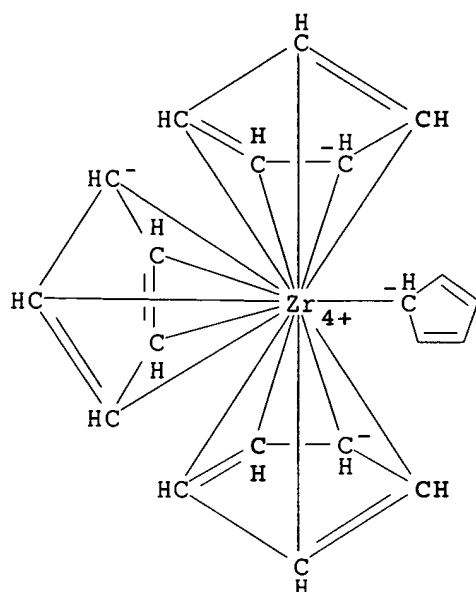
IT 1273-01-4

RL: PRP (Properties)

(NMR and structure of)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 73-4 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)

IT 1273-01-4 1291-32-3 12104-61-9 12116-66-4 33291-92-8

35194-88-8 41433-45-8 56711-97-8

RL: PRP (Properties)
(NMR and structure of)

L31 ANSWER 59 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1973:442642 Document No. 79:42642 Cyclopentadienyl compounds of zirconium and hafnium containing haloacetate ligands. Brainina, E. M.; Bryukhova, E. V.; Lokshin, B. V.; Alimov, N. S. (Inst. Elementoorg. Soedin., Moscow, USSR). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (4), 891-5 (Russian) 1973. CODEN: IASKA6. ISSN: 0002-3353.

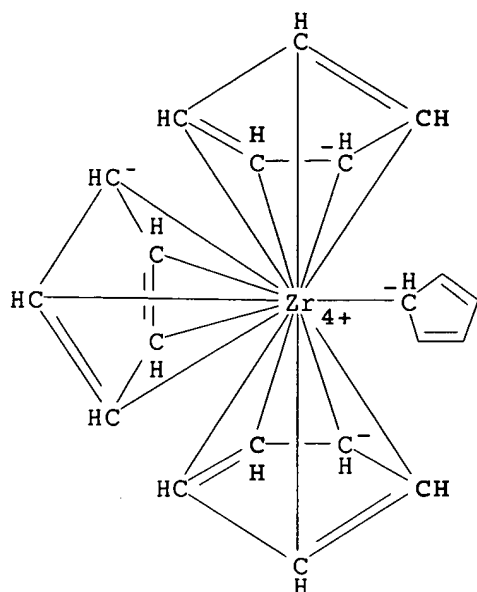
AB Treating tetracyclopentadienyl zirconium or hafnium with chloroacetic acids gave dicyclopentadienylzirconium (or hafnium) diacylates (acyl = O₂CCH₂Cl, O₂CCHCl₂, O₂CCCl₃ or their Br analogs). ³⁵Cl NQR and ir spectra of the products were discussed concerning the nature of binding of the haloacetate groups to the metal. Monodentate bonding exists at the carboxylate groups only, although the trihaloacetates had weak ir bands indicating possible bidentate bonding of the carboxyl groups.

IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with haloacetic acids)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 1273-01-4 12149-28-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with haloacetic acids)

L31 ANSWER 60 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1972:475301 Document No. 77:75301 Preparation of tetracyclopentadienyl zirconium. Medvedeva, A. V.; Ryabenko, D. M. (USSR). Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation), 45(6), 1296-8 (Russian) 1972. CODEN: ZPKHAB. ISSN: 0044-4618.

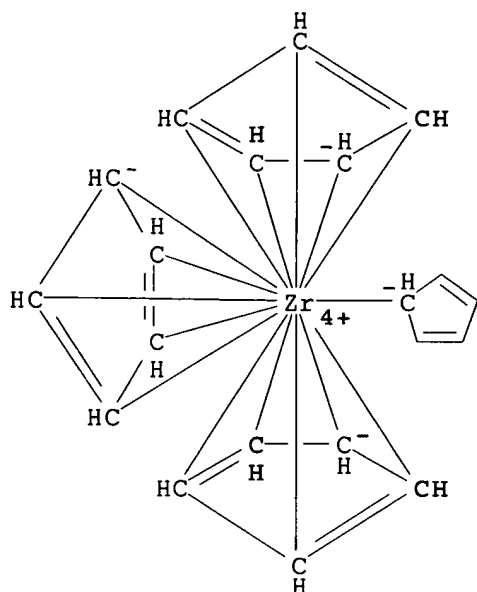
AB Optimum conditions for prepg. the title compd. (I) were: reaction of Na with cyclopentadiene in Et₂O, evapn. of the solvent, and treatment of ZrCl₄ with 6 equiv. of cyclopentadienylsodium in C₆H₆ at room temp. for 2 hr. I sublimed at 200° in vacuo, decompd. at >180°, was sol. in C₆H₆ and PhMe but not in Et₂O, and decompd. slowly in dry air and rapidly in moist air to give mixed cyclopentadienylzirconium hydroxides.

IT 1273-01-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(optimum conditions for prepn. of)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 1273-01-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(optimum conditions for prepn. of)

L31 ANSWER 61 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1972:419770 Document No. 77:19770 Chemical transformations of
tetracyclopentadienylzirconium. Minacheva, M. Kh.; Brainina, E. M.
(Inst. Elementoorg. Soedin., Moscow, USSR). Izvestiya Akademii Nauk
SSSR, Seriya Khimicheskaya (1), 139-43 (Russian) 1972.
CODEN: IASKA6. ISSN: 0002-3353.

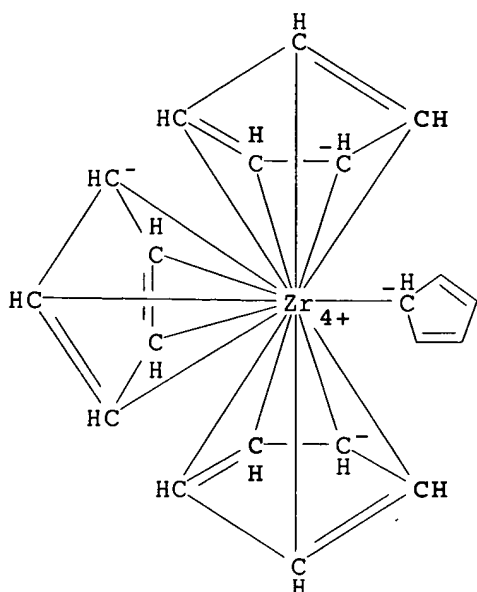
AB (C₅H₅)₄Zr (I) and MeOH in C₆H₆ gave 98% (C₅H₅)₂ZrR₂ (II, R = OMe).
Similarly prepd. were II (R = OPh, OEt SPh). I and CCl₃CO₂H gave
54% (C₅H₅)₂Zr(O₂CCCl₃)₂ (II, R = O₂CCCl₃) and (C₅H₅)₂Zr-(O₂CCCl₃)-
THF complex in THF. CF₃CO₂H and I gave II (R = O₂CCF₃). I and Br
in Cl(CH₂)₂Cl gave 75% (C₅H₅)₂ZrBr₂ (III) and tribromocyclopentene;
in CHCl₃ the product was III also. I and 40% HF gave 21%
(C₅H₅)₂ZrF₂·2O (IV), which with HCl gave (C₅H₅)₂ZrCl₂. Treatment of
IV with CCl₃CO₂H and Ac₂O gave 67% II (R = O₂CCCl₃).

IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with alcs. and acids)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-
yl- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 1273-01-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with alcs. and acids)

L31 ANSWER 62 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1972:419755 Document No. 77:19755 Rapid exchange between nonequivalent cyclopentadienyl rings in tetracyclopentadienyl derivatives of Group IVA metals. Brainina, E. M.; Gambaryan, N. P.; Lokshin, B. V.; Petrovskii, P. V.; Struchkov, Yu. T.; Kharlamova, E. N. (Inst. Elementoorg. Soedin., Moscow, USSR). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1), 187-8 (Russian) 1972. CODEN: IASKA6. ISSN: 0002-3353.

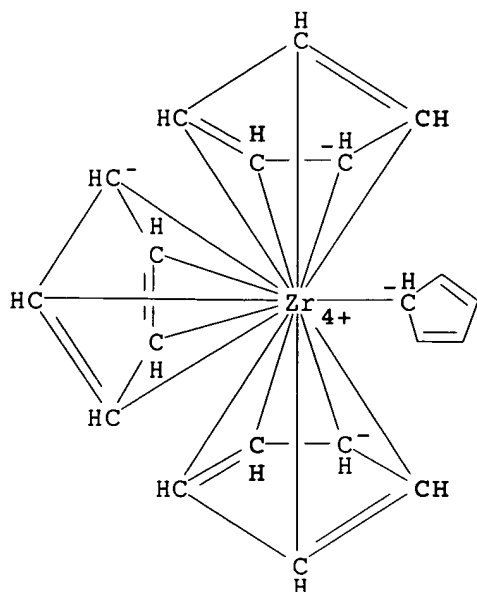
AB X-ray anal. of tetracyclopentadienyltitanium showed 2 monohapto- and 2 pentahapto-cyclopentadienyl rings. The PMR at -27° gave 2 sharp signals (τ 4.82 (π -bound) and τ 4.12 (σ -bound) rings). Increase of temp. caused the signals to widen and merge (indication of facile ring exchange). More facile ring exchange was found among nonequivalently bound rings in tetracyclopenta-dienyl compds. of Zr and Hf; the former had 3 pentahapto bound rings and one monohapto bound ring and the large dipole moment (3.56D) indicated the nonequivalence; yet the PMR even at -150° showed a sharp single signal indicative of facile exchange. The Hf compd. gave similar results but anal. was incomplete.

IT 1273-01-4 11079-32-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(bonding in)

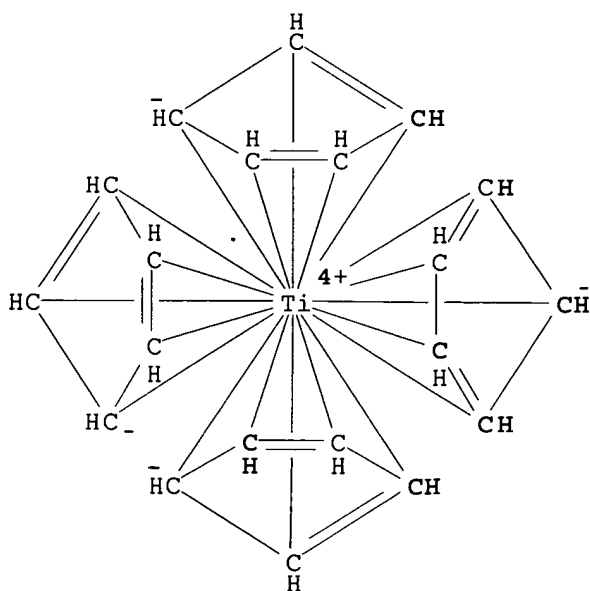
RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



RN 11079-32-6 HCAPLUS

CN Titanium, tetrakis(η5-2,4-cyclopentadien-1-yl) - (9CI) (CA INDEX NAME)



CC 29-8 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 70

IT 1273-01-4 11079-32-6 12149-28-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(bonding in)

L31 ANSWER 63 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1972:98617 Document No. 76:98617 Vibrational spectra and structure of

zirconium and hafnium tetracyclopentadienyl derivatives. Lokshin, B. V.; Brainina, E. M. (Inst. Elementoorg. Soedin., Moscow, USSR). Zhurnal Strukturnoi Khimii, 12(6), 1001-6 (Russian) 1971. CODEN: ZSTKAI. ISSN: 0136-7463.

AB In this abstr., Cp = cyclopentadienyl.) The anal. of ir and vibrational spectra of Cp₄Zr and Cp₄Hf showed the nonequivalence of the Cp rings in cryst. substances. Marked differences between the vibrational spectra of both cryst. compds. proved that their crystals are not isostructural, but there are also probably different chem. structures for both mols. The ir spectra were obtained for cryst. samples and in org. solvents and significantly differentiated one from another with respect to both the no. of bands and their intensity. The structural differences of both the compds., cryst. and in soln. can be connected with different ratios of no. of the h5- and h1-rings in a mol. Other types of the Cp ring-metal bonds and the occurrence of weak metal-ring-double-bond interactions are possible.

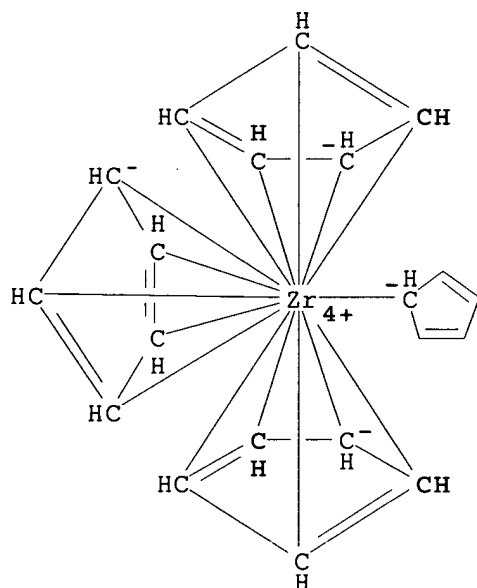
IT 1273-01-4

RL: PRP (Properties)

(vibrational spectrum of, structure in relation to)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 22 (Physical Organic Chemistry)

IT 1273-01-4 12149-28-9

RL: PRP (Properties)

(vibrational spectrum of, structure in relation to)

L31 ANSWER 64 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1971:529910 Document No. 75:129910 Hydrothermal equilibria and crystal growth of rare earth oxides, hydroxides, hydroxynitrates, and hydroxycarbonates. Haschke, John M.; Eyring, LeRoy (Dep. Chem., Arizona State Univ., Tempe, AZ, USA). Inorganic Chemistry, 10(10), 2267-74 (English) 1971. CODEN: INOCAJ. ISSN: 0020-1669.

AB The syntheses of title Th(C₉H₇)₃C and U(C₉H₇)₃Cl are reported.

Evidence is given for the existence of $\text{Th}(\text{C}_9\text{H}_7)_4$, $\text{U}(\text{C}_9\text{H}_7)_4$, $\text{Th}(\text{C}_9\text{H}_7)_2\text{Cl}_2$, and $\text{U}(\text{C}_9\text{H}_7)_2\text{Cl}_2$. Some properties of the triindenylactinide halide complexes are described. Evidence is given for the presence of metal to indenyl ligand bonds with the C5-ring parts of the ligands centrally bonded to the metals. The indenyl to uranium bonds is more covalent in character than the indenyl to thorium bond.

IT 11082-82-9

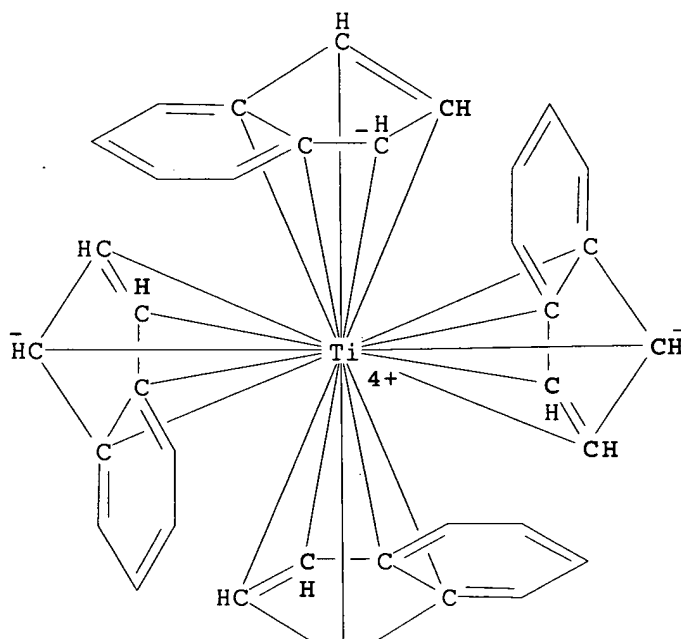
RL: PRP (Properties)

(mass spectrum of)

RN 11082-82-9 HCAPLUS

CN Uranium, tetra- π -indenyl- (8CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



CC 29 (Organometallic and Organometalloidal Compounds)

IT 11082-82-9 11133-17-8, Thorium, tetra- π -indenyl-

RL: PRP (Properties)

(mass spectrum of)

L31 ANSWER 65 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1971:482236 Document No. 75:82236 Stereochemically nonrigid organometallic molecules. XXVII. Fluxional behavior of tetra(cyclopentadienyl)titanium. Cotton, F. A.; Calderon, J. L.; Takats, J. (Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, USA). Journal of the American Chemical Society, 93(15), 3587-91

(English) 1971. CODEN: JACSAT. ISSN: 0002-7863.

AB The temp. dependence of the NMR spectrum of $\text{Ti}(\text{C}_5\text{H}_5)_4$ from +80 to -140° has been studied. The observations can be explained by assuming that the mol. is $(\text{h}1\text{-C}_5\text{H}_5)_2(\text{h}5\text{-C}_5\text{H}_5)_2\text{Ti}$ and that it executes 2 types of intramol. rearrangement. At the lowest temps. of observation the $\text{h}1\text{-C}_5\text{H}_5$ rings rotate relatively slowly but by about -25° averaging is rapid enough to give a single line as narrow as that for the protons of the $\text{h}5\text{C}_5\text{H}_5$ rings. Between about -20 and +35° the sep. $\text{h}1\text{-C}_5\text{H}_5$ and $\text{h}5\text{-C}_5\text{H}_5$ lines broaden and coalesce to a single line which continues to become narrower as the temp. is raised further. These changes are attributable to interchange of the $\text{h}1\text{-C}_5\text{H}_5$ and $\text{h}5\text{-C}_5\text{H}_5$ types of rings and this is the 1st known observation of such an interchange. The activation parameters are: $E_a = 16.1 \pm 0.3$ kcal/mole and $\log A = 13.5 \pm 0.5$. The relatively ready occurrence of this heretofore unknown process is attributable to the presence of an empty valence-shell orbital on the Ti atom of $(\text{h}1\text{-C}_5\text{H}_5)_2(\text{h}5\text{-C}_5\text{H}_5)_2\text{Ti}$ which makes a reasonably low-lying transition state accessible. The $(\text{C}_5\text{H}_5)_3\text{TiCl}$ mol. has been obsd. by PMR in soln. It shows a single sharp line down to at least -100°.

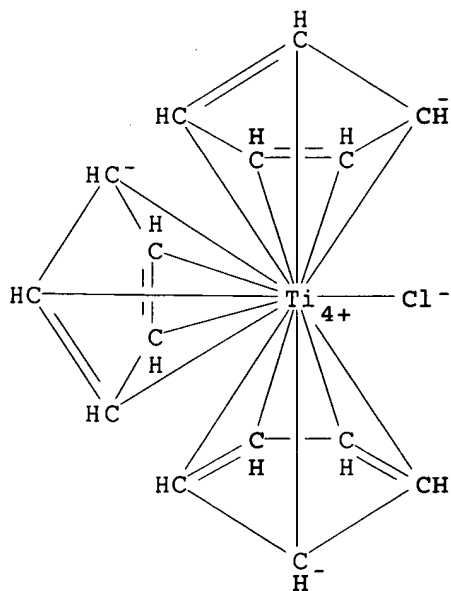
IT 11079-20-2 11079-32-6

RL: PRP (Properties)

(nuclear magnetic resonance of, ring interchange in relation to)

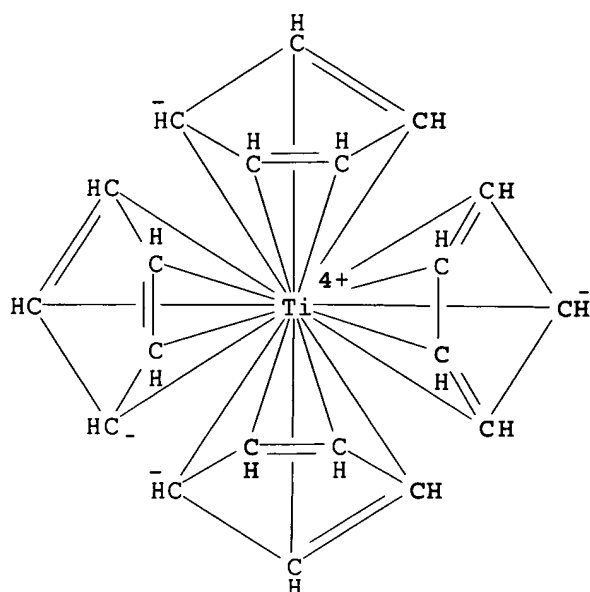
RN 11079-20-2 HCAPLUS

CN Titanium, chlorotris($\eta^5\text{-2,4-cyclopentadien-1-yl}$)- (9CI) (CA INDEX NAME)



RN 11079-32-6 HCAPLUS

CN Titanium, tetrakis($\eta^5\text{-2,4-cyclopentadien-1-yl}$)- (9CI) (CA INDEX NAME)



CC 73 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)

IT 11079-20-2 11079-32-6

RL: PRP (Properties)

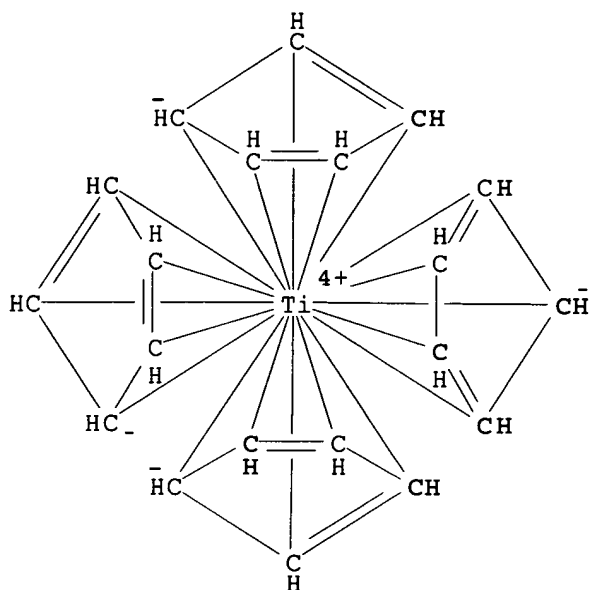
(nuclear magnetic resonance of, ring interchange in relation to)

L31 ANSWER 66 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1971:481377 Document No. 75:81377 Stereochemically nonrigid organometallic molecules. XXVIII. Crystal and molecular structures of tetra(cyclopentadienyl)titanium. Cotton, F. A.; Calderon, J. L.; DeBoer, B. G.; Takats, J. (Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, USA). Journal of the American Chemical Society, 93(15), 3592-7 (English) 1971. CODEN: JACSAT. ISSN: 0002-7863.

AB The crystal and mol. structures of $(C_5H_5)_4Ti$ have been detd. from 1205 reflections, including 384 Friedel pairs, collected with a counter diffractometer. The compd. crystallizes in the hexagonal space group $P6_122$ with 6 mols., each lying on a 2-fold axis of rotation, in a unit cell of dimensions $a = b = 9.214 \pm 0.003$ Å, $c = 21.895 \pm 0.006$ Å ($\rho_{calcd} = 1.31$ g cm $^{-3}$). The structure, including H atoms, was solved from Patterson and electron-d. maps and refined by least-squares methods to a conventional unweighted R factor of 3.6%. The structure shows unambiguously that the mol. contains 2 pentahapto- and 2 monohaptocyclopentadienyl rings ($h^5-C_5H_5$ and $h^1-C_5H_5$, resp.); the metal atom, therefore, has a 16-electron configuration. The distance from the $h^5-C_5H_5$ ring center to the Ti atom is 2.078 Å; individual Ti-C distances (Å) are: 2.381(4), 2.359(4), 2.373(3), 2.391(4), 2.400(5). The other C_5H_5 ring is an exemplary monohaptocyclopentadienyl ring. The Ti-C distance is 2.332(2) Å, and the C-C distances (Å), listed in order from the bound C atom around the ring, are: 1.446(5), 1.360(6), 1.420(5), 1.355(6), and 1.442(3). The findings reported here lend considerable support to our claim that $(C_5H_5)_4Ti$ provides the 1st genuine example of the occurrence of rapid interchange of $h^1-C_5H_5$ and $h^5-C_5H_5$ rings as part of the fluxional behavior of the mol.

IT 11079-32-6
 RL: PRP (Properties)
 (crystal structure of)
 RN 11079-32-6 HCAPLUS
 CN Titanium, tetrakis(η^5 -2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



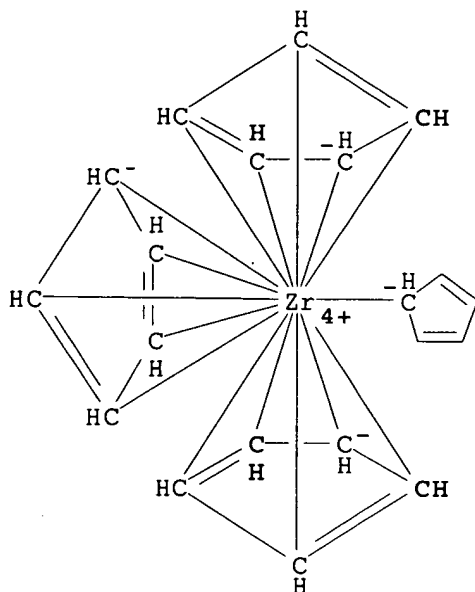
CC 70 (Crystallization and Crystal Structure)
 IT 11079-32-6
 RL: PRP (Properties)
 (crystal structure of)

L31 ANSWER 67 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1971:104390 Document No. 74:104390 Dipole moments of some cyclopentadienyl compounds of zirconium and hafnium. Kharlamova, E. N.; Brainina, D. M.; Gur'yanova, E. N. (Inst. Elementoorg. Soedin., Moscow, USSR). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (11), 2621-2 (Russian) 1970. CODEN: IASKA6. ISSN: 0002-3353.

AB The following values of dipole moments were detd. from dielec. data in C₆H₆ at 25°: (C₅H₅)₄Zr, 3.41; at 50°, 3.57; (C₅H₅)₄Hf, 3.76; (C₅H₅)₂ZrCl₂ (I), 4.87; (C₅H₅)₂HfCl₂, 4.66; C₅H₅ZrCl(C₅H₇O₂)₂, 5.71; its Hf analog, 5.81; [C₅H₅Zr(C₅H₇O₂)]₂O, 3.63 D (C₅H₇O₂ = acetylacetone residue). The acetylacetone derivs. evidently have the octahedral cis configuration at room temp., while the structure of I and its Hf analog is tetrahedral with angular position of the cyclopentadiene rings, which are joined by a central σ bond. The R₄M-type compds. above probably have structures that are not sym., and probably are similar to those suggested by x-ray anal.

IT 1273-01-4
 RL: PRP (Properties)
 (dipole moment of)
 RN 1273-01-4 HCAPLUS
 CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 71 (Electric Phenomena)

IT 1273-01-4 1291-32-3 11058-81-4 12116-66-4 12147-78-3
 12149-28-9 12216-18-1
 RL: PRP (Properties)
 (dipole moment of)

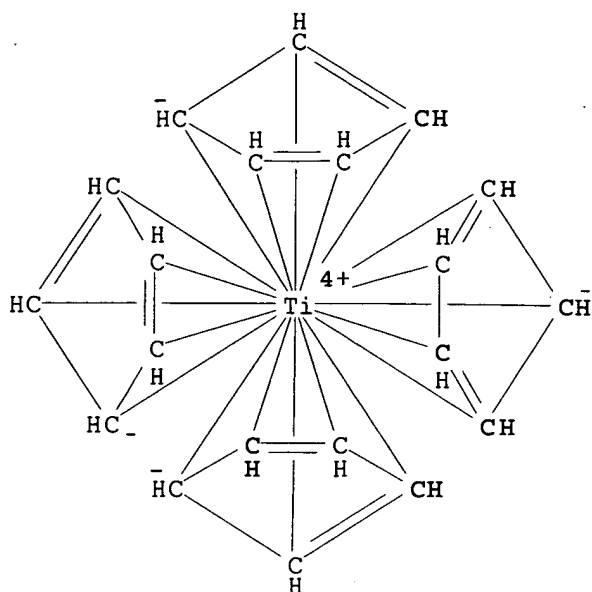
L31 ANSWER 68 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN
 1970:31969 Document No. 72:31969 Tetracyclopentadienyltitanium(IV) and
 tricyclopentadienyltitanium(III). Siegert, F. W.; De Liefde Meijer,
 H. J. (Rijksuniv., Groningen, Neth.). Journal of Organometallic
 Chemistry, 20(1), 141-5 (English) 1969. CODEN: JORCAI.
 ISSN: 0022-328X.

AB The syntheses and properties of the complexes $(C_5H_5)_4Ti$ and
 $(C_5H_5)_3Ti$ are described. Ir and NMR spectra show that these
 complexes have the structures $(\pi-C_5H_5)_2-Ti(\sigma-C_5H_5)_2$ and
 $(\pi-C_5H_5)_2Ti(\sigma-C_5H_5)$ resp. The spectra and properties of
 the two compds. are compared with those of $(\pi-C_5H_5)_2Nb(\sigma-$
 $C_5H_5)_2$ and $(\pi-C_5H_5)_2V(\sigma-C_5H_5)$. The compd.
 $(\pi-C_5H_5)_2V(\sigma-C_5H_5)_2$ could not be prepd.

IT 11079-32-6P, Titanium, di- π -cyclopentadienyldi-2,4-
 cyclopentadien-1-yl-
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 11079-32-6 HCAPLUS

CN Titanium, tetrakis(η^5 -2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX
 NAME)



CC 29 (Organometallic and Organometalloidal Compounds)

IT 1277-47-0P 11079-32-6P, Titanium, di- π -
cyclopentadienyldi-2,4-cyclopentadien-1-yl-
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L31 ANSWER 69 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1969:475262 Document No. 71:75262 Unit cells and space groups of
zirconium and hafnium cyclopentadienyl compounds. Sudarikov, V. S.;
Kulishov, V. I.; Bokii, N. G.; Struchkov, Yu. T. (Inst. Elementoorg.
Soedin., Moscow, USSR). Zhurnal Strukturnoi Khimii, 10(3), 558
(Russian) 1969. CODEN: ZSTKAI. ISSN: 0136-7463.

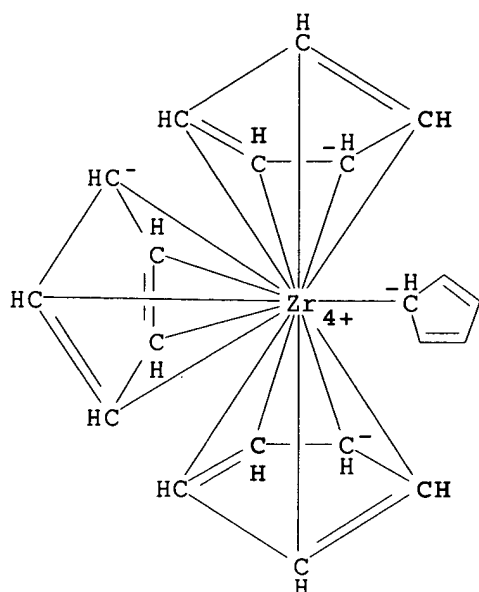
AB Results of preliminary x-ray diffraction studies of
(C₅H₇O₂)₂C₅H₅ZrCl, (C₅H₇O₂)₂(C₅H₅)HfCl, and (C₅H₅)₄Zr are presented.
The crystals have a 8.40, 8.67, 20.64; b 15.60, 15.33, 8.38; c
14.92, 14.85, 8.61; β 123.5°, 124°, -; space
groups are P2₁/c, P2₁/c, Pna2 or Pnam, resp. Z = 4 for all 3. A
complete analysis will be made in the near future.

IT 1273-01-4

RL: PRP (Properties)
(crystal structure of)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-
yl- (9CI) (CA INDEX NAME)



CC 70 (Crystallization and Crystal Structure)

IT 1273-01-4 12147-78-3, Hafnium, chloro- π -cyclopentadienylbis(2,4-pentanedionato)- 12216-18-1, Zirconium, chloro- π -cyclopentadienylbis(2,4-pentanedionato)-
 RL: PRP (Properties)
 (crystal structure of)

L31 ANSWER 70 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1967:421990 Document No. 67:21990 Tetracyclopentadienylzirconium. Brainina, E. M.; Dvoryantseva, G. G. (Int. Elementoorgan. Soedin., Moscow, USSR). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (2), 442-3 (Russian) 1967. CODEN: IASKA6. ISSN: 0002-3353.

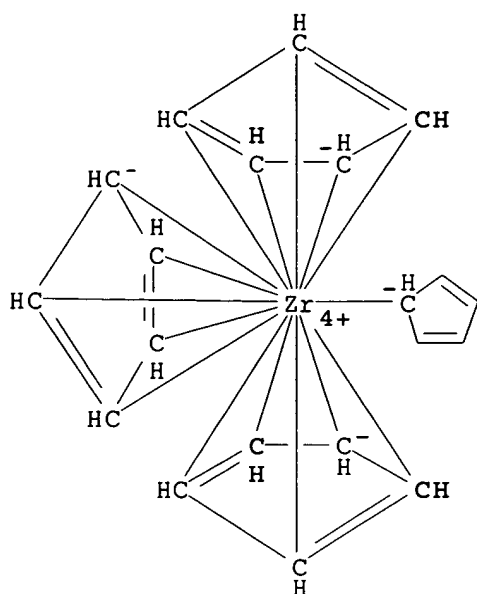
AB Tetracyclopentadienylzirconium (I), cryst. solid from C_6H_6 , formed in 69% yield from dicyclopentadienylzirconium dichloride and C_5H_5Na in MePh, was characterized by ir spectrum and proton N.M.R. spectrum (reported). The stability of I was examd. thermogravimetrically to 75° at which it was still stable in air, but at higher temps. decompd. vigorously, losing up to 4% of its wt. in air at 150°, while further loss to 40% of initial wt. took place at 500°. Heated in dry N, I did not undergo a vigorous decompn. but slowly lost wt. at 400-600° with declines of 40-60%. Thus I has low hydrolytic stability. The spectra of I showed the absence of ligands of the diene type; all protons were equiv. as were all the metal-ring bonds.

IT 1273-01-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 29 (Organometallic and Organometalloidal Compounds)

IT 1273-01-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L31 ANSWER 71 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1966:482395 Document No. 65:82395 Original Reference No.

65:15421g-h,15422a Cyclopentadienyl compounds of zirconium containing chelate groups. Brainina, E. M.; Mortikova, E. I.; Petrashkevich, L. A.; Freidlina, R. Kh. (Inst. Heteroorg. Compds., Moscow). Doklady Akademii Nauk SSSR, 169(2), 335-8 (Russian) 1966. CODEN: DANKAS. ISSN: 0002-3264.

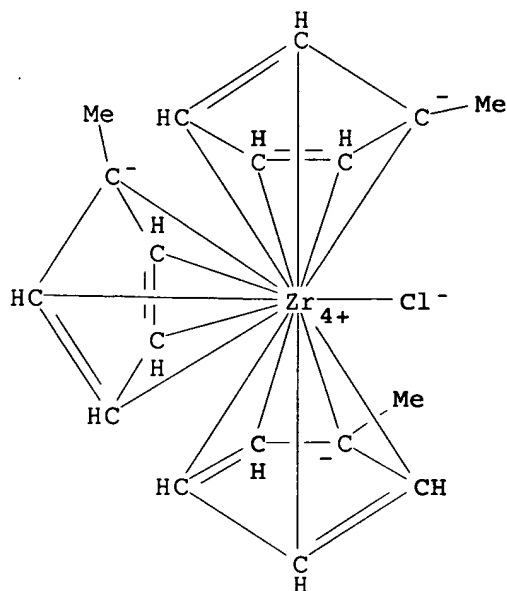
AB Dicyclopentadienylzirconium dichloride and 8-hydroxyquinoline (I) in C₆H₆ 20 min. at 80° gave a ppt. of I.HCl while the filtrate yielded 51% tris(8-quinolinoxy)cyclopentadienylzirconium (II), decompd. at 357-60°, which formed an adduct with CHCl₃. II was also formed from dicyclopentadienyldizirconoxane tetraacetylacetonate and I in 1.5 hrs. at 100° or from tetracyclopentadienylzirconium and I at 70-80° in C₆H₆. The latter method with Bz₂CH₂ gave tris(dibenzoylmethanate) of cyclopentadienylzirconium C₅H₅Zr(C₁₅H₁₁O₂)₃, m. 186-7°, while BzCH₂Ac similarly gave in 2 hrs. at room temp. 52% cyclopentadienylzirconium tribenzoylacetonate, m. 141-2°. Similarly, Ac₂CH₂ gave 100% oily cyclopentadienylzirconium triacetylacetonate which in contact with moisture gave dicyclopentadienyldizirconoxane tetraacetylacetonate, m. 163-4°. Addn. of 1.1 g. ZrCl₄ to Na methylcyclopentadienide from 1.5 g. Na and 4 ml. methylcyclopentadiene in MePh under argon gave in 3 hrs. yellow tris(methylcyclopentadienyl)zirconium chloride decompd. at 168-70°, which was extremely hygroscopic. This and I under Ar in C₆H₆ gave 60% methylcyclopentadienylzirconium tris-8-quinolinoxy, decompd. at 252-60°.

IT 12095-84-0, Zirconium, chlorotris(methylcyclopentadienyl)-
(prepn. of)

RN 12095-84-0 HCAPLUS

CN Zirconium, tris(η⁵-2,4-cyclopentadien-1-yl)-, chloride (9CI)

(CA INDEX NAME)



CC 39 (Organometallic and Organometalloidal Compounds)
 IT 5381-89-5, 2,3-Butanediol, 1-phenyl-, zirconium complex
 12095-84-0, Zirconium, chlorotris(methylcyclopentadienyl)-
 12102-42-0, Zirconium, tris(8-quinolinolato)cyclopentadienyl-
 12102-60-2, Zirconium, tris(8-quinolinolato)(methylcyclopentadienyl)-
 12104-61-9, Zirconium, tris(1,3-diphenyl-1,3-propanedionato)cyclopentadienyl- 12118-83-1, Chloroform, compd.
 with tris(8-quinolinolato)cyclopentadienylzirconium (1:1)
 59370-57-9, 1,3-Propanedione, 1,3-diphenyl-, zirconium complex
 (prepn. of)

L31 ANSWER 72 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

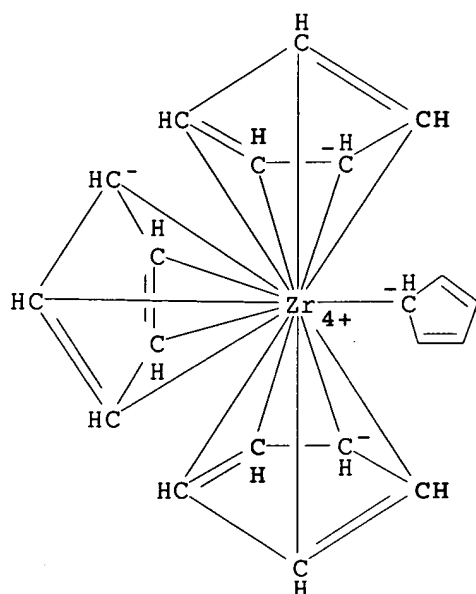
1966:19502 Document No. 64:19502 Original Reference No. 64:3594b-c
 Some properties of tetracyclopentadienylzirconium. Brainina, E. M.;
 Minacheva, M. Kh.; Freidlina, R. Kh. (Inst. Heteroorg. Compds.,
 Moscow). Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (10),
 1877-9 (Russian) 1965. CODEN: IASKA6. ISSN: 0002-3353.

AB Na cyclopentadienide and dicyclopentadienylzirconium dichloride in
 C6H6 gave in 5 hrs. 54% (C5H5)4Zr (I), a solid. This and H2O in 2.5
 hrs. at 100° gave C5H5 and ZrO2. EtOH at 95° gave 86%
 C5H5 and 71% (EtO)4Zr. HCl at 25° gave (C5H5)2ZnCl2, m.
 238-9°. I and HNO3 (d. 1.34) in (CH2Cl)2 at -35°,
 then at room temp., gave 67% (C5H5)2Zn(NO3)2, explodes at
 185°. I and BzOH in tetrahydrofuran at -10° to room
 temp. gave 45% [(C5H5)x(BzO)2Zr]2O, contg. 3 moles tetrahydrofuran,
 an infusible solid. This and BzOH in C6H6 gave 45% C5H5Zr(OBz)3
 monohydrate, m. 126-7°. I and ZrCl4 in tetrahydrofuran gave
 at 40° in 6 hrs. 34% (C5H5)2ZrCl2.

IT 1273-01-4, Zirconium, tetracyclopentadienyl-
 (prepn. and properties of)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η5-2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 39 (Organometallic and Organometalloidal Compounds)

IT 1273-01-4, Zirconium, tetracyclopentadienyl-
(prepn. and properties of)

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1966:19501 Document No. 64:19501 Original Reference No.

64:3593h,3594a-b Direct methylenation of 1-substituted cyclopentenes and -hexenes. Shabarov, Yu. S.; Surikova, T. P.; Svirina, V. S.; Levina, R. Ya. (State Univ., Moscow). Zhurnal Obshchei Khimii, 1(10), 1895-6 (Russian) 1965. CODEN: ZOKH44. ISSN: 0044-460X.

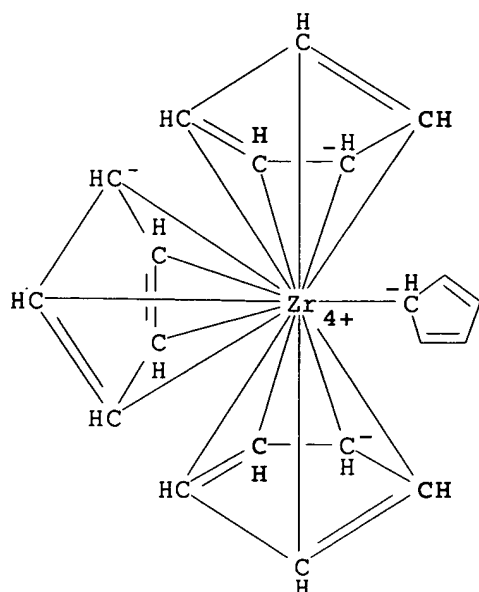
GI For diagram(s), see printed CA Issue.

AB Reaction of appropriate 1-substituted cyclopentenes and cyclohexenes with CH_2I_2 in the presence of Zn-Cu couple (for best prepn. LeGoff (CA 61, 9411g)) gave: 38% 1-methylbicyclo[0.1.3]hexane, b. $91-2^\circ$, n_{D}^{20} 1.4327, d_{20} 0.8116; 33% 1-methylbicyclo[0.1.4]heptane, b. $124-5^\circ$, 1.4498, 0.8344; 56% 1-phenylbicyclo[0.1.3]hexane, b3 $93-4^\circ$, 1.5482, 0.9954; 66% 1-phenylbicyclo[0.1.4]heptane, b3 $104-5^\circ$, 1.5425, 0.9968. These and $\text{Hg}(\text{OAc})_2$ gave the following 1-R-substituted-2-acetoxymethylmercurimethylcycloalkanols (I) (R and n shown): Me, 3, m. $70-1^\circ$; Ph, 3, -- (oil); Me, 4, m. $103-4^\circ$; Ph, 4, m. $143-6^\circ$.

IT 1273-01-4, Zirconium, tetracyclopentadienyl-
(prepn. and properties of)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-yl- (9CI) (CA INDEX NAME)



CC 39 (Organometallic and Organometalloidal Compounds)

IT 1273-01-4, Zirconium, tetracyclopentadienyl-
(prepn. and properties of)

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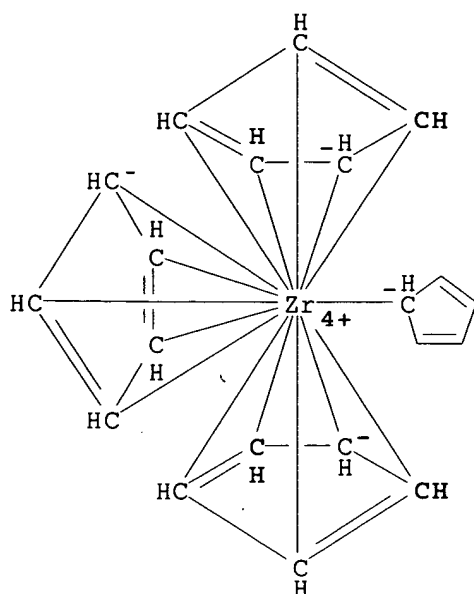
1965:49366 Document No. 62:49366 Original Reference No. 62:8713b-c
Zirconium tetracyclopentadienyl. Medvedeva, A. V.; Ryabenko, D. M.;
Zayarnaya, R. F.; Fridenberg, A. E. (Organization of the State
Committee for the Chemical Industry under the State Planning
Committee of the Council of Ministers of the U.S.S.R.). SU 166689
19641201 From: Byul.-Izobret. i Tovarnykh Znakov 1964(23),
22.. (Unavailable). APPLICATION: SU 19631229.

AB The title compd. is prepd. from the reaction of Na cyclopentadiene
with $ZrCl_4$ in an inert org. solvent in an atm. of N.

IT 1273-01-4, Zirconium, tetracyclopentadienyl-
(manuf. of, from cyclopentadiene, Na and $ZrCl_4$)

RN 1273-01-4 HCAPLUS

CN Zirconium, tris(η^5 -2,4-cyclopentadien-1-yl)-2,4-cyclopentadien-1-
yl- (9CI) (CA INDEX NAME)



IC C07F
 CC 17 (Industrial Inorganic Chemicals)
 IT 1273-01-4, Zirconium, tetracyclopentadienyl-
 (manuf. of, from cyclopentadiene, Na and ZrCl₄)

L31 ANSWER 75 OF 75 HCAPLUS COPYRIGHT 2006 ACS on STN

1963:462549 Document No. 59:62549 Original Reference No.

59:11557h,11558a-b Cyclopentadienyl-and diethyl malonate titanium compounds. Breederveld, Heyme; Waterman, Hein I. (Shell Oil Co.).

US 3089886 19630514, 3 pp. (Unavailable). PRIORITY: GB 19520505.

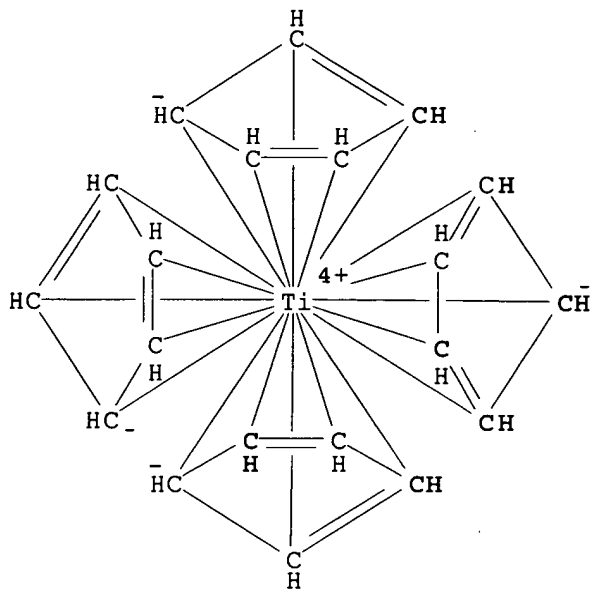
AB Reaction of TiCl₄ (I) with K cyclopentadiene gives a tetracyclopentadienyltitanium. Reaction of I with the sodio deriv. of diethyl malonate (II) gives diethyl malonate titanium compds. The products are useful for water-proofing, and for making catalysts and surface coatings. To a dispersion of 58.5 g. K in 1200 ml. C₆H₆ maintained at 15° was added a soln. of 99 g. cyclopentadiene in 400 ml. of C₆H₆ during 2 hrs. The mixt. was heated to boiling for a short time, cooled, and kept at 15° while 64.2 g. I in 160 ml. of C₆H₆ was added during 1 hr. The solvent was removed in vacuo, 1 l. of Et₂O added, the brown soln. decanted from the KCl produced, and evapd. to give impure, brown, partly polymeric tetracyclopentadienyltitanium. To a soln. of 109.5 g. II in 700 ml. C₆H₆ was added 14 g. Na wire, the mixt. refluxed 5 hrs., cooled, a soln. of 29 g. I in 60 ml. of C₆H₆ added during 30 min., the mixt. refluxed 45 min., volatile materials removed by distn. at 50-60°/80 mm. and the pasty residue extd. with 0.5 l. Et₂O. The ext. was evapd. to give a pasty red product, which contained little Cl, and was a mixt. of diethyl malonate titanium compds., of mol. wt. about 720, contg. 10.5% of Ti, and with about 2.4 diethyl malonate groups/Ti atom. A soln. of 182 g. diethyl sodiomalonate in 600 ml. C₆H₆ was added during 1 hr. to a stirred soln. of 190 g. I in 400 ml. C₆H₆. Volatile materials were removed in vacuo, and then at 120°/22 mm. for 1 hr. The residue was extd. with 1 l. boiling Et₂O for 3 hrs., and the ext. decanted. The Et₂O was removed at 10° in vacuo and the residue heated at

125°/2 mm. to yield 17.5 g. of a hard, glassy, brown mass of $\text{Cl}_3\text{TiCH}(\text{CO}_2\text{Et})_2$.

IT 11079-32-6, Titanium, tetracyclopentadienyl-
(prepn. of)

RN 11079-32-6 HCAPLUS

CN Titanium, tetrakis(η^5 -2,4-cyclopentadien-1-yl)- (9CI) (CA INDEX NAME)



INCL 260429500

CC 39 (Organometallic and Organometalloidal Compounds)

IT 976-28-3, Borazine, 2,4,6-triphenyl- 11079-32-6, Titanium,
tetracyclopentadienyl- 875217-52-0, Titanium,
dichlorobis(dicarboxymethyl)-, tetraethyl ester
(prepn. of)

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